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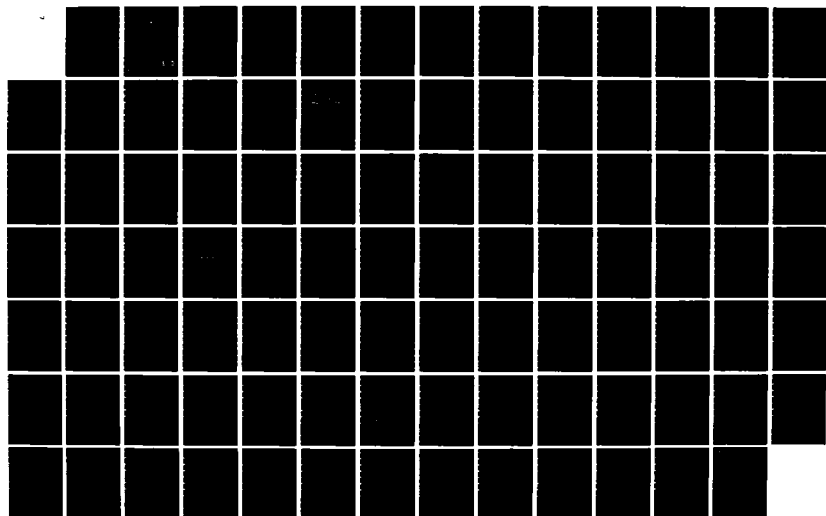
SOLITON PROPAGATION IN ONE-DIMENSIONAL ORGANIC
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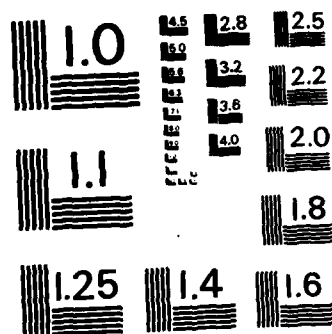
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SOLITON PROPAGATION IN ONE-DIMENSIONAL ORGANIC CONDUCTORS

T.W. Barrett
Naval Air Systems Command
Department of the Navy
Washington, D.C. 20361

SEPTEMBER 1983

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20. (Continued)

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SUMMARY

Criteria are stated for the existence of solitons in one-dimensional organic conductors, particularly trans polyacetylene. All physical situations considered are described in terms of a classical anharmonic oscillator moving in an anharmonic double potential well. As the soliton is known to exist in the line of pendula joined with elastic coupling and also in the long Josephson junction in the form of the fluxon, the theoretical position is taken that if, indeed, the soliton exists in polymers, whether of the vibrational or the charge-domain-wall-type, then it should conform to certain established criteria of behavior already rigorously studied in the aforementioned situations.

In order to understand the dynamics of a conducting one-dimensional system, whether of charge or mechanical energy, a microscopic parametric excitation model formalism must be adopted. On the other hand, in order for this model to be related to physical measurements such as that of current and voltage, a microscopic formalism (the Hubbard model) must also be achieved. Both pictures have advantages and disadvantages. However, both pictures are necessary for complete understanding.

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SOLITON PROPAGATION IN ONE-DIMENSIONAL ORGANIC CONDUCTORS

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I. PRELIMINARIES

The notion of a propagating soliton is not a simple notion and the requirements for its existence are rigorous. The aim of this paper is to indicate the complexity involved in its existence and to suggest criteria for such existence. Another aim is to indicate the fundamental importance of the concept of soliton, first called such in 1965 (Zabusky and Kruskal, 1965; Zabusky, 1981), but whose origins stem from observations by John Scott Russell (1834). The timeliness of this endeavor is due to the consideration being given, on the one hand; to proteins (Davydov, 1977-1979; Scott, 1981; Hyman et al., 1981) and deoxyribonucleic acid, DNA, (Balanovski and Beaconsfield, 1982) as mediators of vibrational-type solitons, and, on the other hand, to trans polyacetylene, $(CH)_x$, as a mediator of soliton dependent electrical conductivity or charge-domain-wall movement (Su, Schrieffer and Heeger, 1979, 1980).

The charge-domain-wall-type soliton of $(CH)_x$ has received much attention. The case for the existence of such solitons in $(CH)_x$ has been made mainly on the basis of electron spin resonance (ESR) data (Heeger and MacDiarmid, 1981). That solitons do, in fact, exist in trans polyacetylene could be treated as a hypothesis. On the other hand, the mathematical entity of the soliton has undergone considerable evolution and its history has been described by Scott (1981). The intention, here, is not to question whether the mathematical entity of soliton propagation can exist in polymers (undoubtedly it does) but to refine judgment concerning when it can and

when it cannot. This is a matter of discrimination based on both physical and mathematical reasoning.

All physical situations considered here are described in terms of a classical anharmonic oscillator moving in an anharmonic double potential well (DPW). As the soliton is known to exist in the line of pendula joined with elastic coupling and also in the long Josephson junction as the fluxon, the attitude has been taken here that if, indeed, the soliton exists in polymers, whether of the vibrational or charge-domain-wall-type, then it should conform to certain established criteria of behavior already rigorously studied in the aforementioned situations.

The main theme, here, is that in order to understand the dynamics of a conducting one-dimensional system, whether of charge or mechanical energy, a microscopic parametric excitation model formalism must be first achieved (sections I-IX). On the other hand, in order for this model to be related to physical measurements such as that of current and voltage, a macroscopic formalism (using the Hubbard model) must also be achieved (sections X-XI). Both pictures have advantages and disadvantages. However, both pictures are necessary for a complete understanding.

In section III, the possibility of sending solitons through joined one-dimensional chains into one arm or both arms of a T-junction is examined. The conclusion of this section is: if it were possible to synthesize a polymer made up of joined segments (of CH_x for example) the synthesized polymer would demonstrate different phonon modes in the vicinity of the junction, due to different phonon-dependent propagation energies. The likelihood is that the soliton would not progress past the junction into the arms and probably would not approach within the vicinity of the junction.

In section IV the concept of tunneling is related to a parametric excitation dynamic. The advantage in this is the subsumption of tunneling

behavior under energy conservation rules, rather than probabilistic laws. This aim is of importance, because the mathematical entity of the soliton is itself rigorously restrained by conservation of energy laws (Bullough and Caudrey, 1980).

In section V the effect of pinning solitons is addressed. This amounts to the trapping of a discommensuration so that it is no longer moving. Thus by pinning, a soliton ceases to exist (because it is a dynamic and moving wave by definition) and the resulting static discommensuration, or kink, takes its place. The research literature has sometimes not distinguished between a soliton, which is a moving wave, and a trapped or pinned discommensuration, which is a kink.

In section VI the energy conservation laws for the order parameter, energy and damping constant derived for nonlinear systems, are used to characterize the four forms Ohm's and Kirchoff's laws would take in such nonlinear or soliton exhibiting systems.

In section VII the dynamic form factor or spectral density is introduced which, for a system in a displacive transition mode such as a soliton exhibiting system, contains a soft phonon which pumps the displacement. It may be emphasized that such a concept is out of consideration in a static or even a many body approximation approach to one-dimensional conduction. The dynamic form factor does not even appear in the macroscopic landscape. In treating the dynamic form factor the advantage of a monomer or microscopic treatment of solitons is thus demonstrated. However, in section XI and XII this microscopic treatment is relinquished for a macroscopic or Hubbard many body approximation so that long chain systems may be treated. The dynamic form factor's soft phonon mode remains a facet of soliton existence criteria and of the microscopic approach.

In section VIII the necessary and sufficient conditions for soliton propagation are addressed. Section IV contains a description of soliton propagation in a system of changing and incomplete degeneracy. A system capable of demonstrating soliton propagation is shown in section X to be one in which the equation of motion for the system exhibits broken symmetry. This relation is described in terms of renormalization group theory.

Finally, in section XI a macroscopic picture (the Hubbard model) is introduced and related to the double potential well (DPW) anharmonic oscillator model.

II. INTRODUCTION

It is well known that the interplay of currents and voltages in Josephson circuitry is similar in form to that encountered in certain mechanical systems, and, in particular, to the simple pendulum. The ability to understand and visualize the behavior of Josephson junctions in terms of mechanical devices has greatly facilitated understanding (Fulton 1975, 1977). As (a) the fluxon of the long Josephson junction is a soliton propagation, and (b) the soliton-with-spin and the soliton-with-charge have been implicated in conduction experiments on undoped and doped trans-polyacetylene, the methods used to study the Josephson junction fluxon are readily applicable to the study of the polyacetylene soliton, if it exists. The suggestion that vibrational solitons exist in proteins and DNA may also be studied from this theoretical platform.

The models constructed for the study of the Josephson effect include those of Scott (1969), Waldram et al. (1970), Sullivan and Zimmerman (1971), Yamashita et al. (1974) and Fulton (1977). These models have been of great use in developing physical intuition concerning the effect and agree in their choice of mathematical and physical description of that effect. This

agreement means that actual physical model building is no longer necessary for predicting new behavior and analysis may proceed by numerical methods based on those models.

The advantages of numerical analysis based on mechanical models are many. Firstly, the performance of the model can be readily altered by a change of variables. By dimensional analysis polymer compounds for possible synthesis may be suggested. This approach is more systematic than the trial-and-error method of obtaining compounds by difficult synthesis procedures, testing them and then attempting to explain their function.

Secondly, recent theoretical approaches to the polyacetylene soliton emphasize the static aspects of the problem, obscuring the dynamic and diffusive aspects. An analysis based on a physical explanation refocuses attention on these neglected aspects of the problem.

Thirdly, there are a number of variables of soliton propagation indicated by mechanical analysis which are, as yet, unstudied.

The known and agreed upon conditions for fluxon (soliton) propagation are now examined in the long Josephson junction, and these are used to stipulate the proper conditions for the appearance of solitons in polymers. The rationale for this theoretical posture is that the fluxon (soliton) in the long Josephson junction is firmly established, but the polymer soliton is presently a theoretical inference. The soliton being a mathematical entity, at a level of abstraction, the conditions pertaining to the former soliton (the fluxon) must also apply to the latter (the soliton in polymers, whether vibrational or moving charge wall). Examination of the soliton of the simple pendulum line is also instructive in that its behavior is described in familiar physical variables. Thus, the intention is to prop the theoretical conditions for polymer soliton propagation upon the

established conditions for soliton propagation in the long Josephson junction and the pendulum line.

The phenomenological equations describing the macroscopic behavior of superconducting barriers are (Josephson, 1965):

$$\partial\phi/\partial x = (2ed/\hbar c)H_y; \quad \partial\phi/\partial t = (2e/\hbar)V; \quad J_z = j_1 \sin\phi + \sigma V, \quad (1)$$

where ϕ is the phase difference between two superconductors, H is the magnetic field in the barrier, V is the voltage across the barrier, $d = 2\lambda + \ell$, λ is the penetration depth and ℓ is the barrier thickness. If the barrier is regarded as having a capacitance C per unit area and using Maxwell's equations and Equ.s (1), above, we obtain

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{\bar{c}^2} \frac{\partial^2}{\partial t^2} - \frac{\beta}{\bar{c}^2} \frac{\partial}{\partial t} \right) \phi = \frac{1}{\lambda_0^2} \sin\phi \quad (2)$$

where $\bar{c}^2 = c^2/4\pi dC$ is the phase velocity in the barrier, $\lambda_0^2 = \hbar c^2/8\pi e d j_1$ is the penetration depth, and $\beta = 4\pi d \bar{c}^2 \sigma / c^2 = \sigma/C$ is a damping constant.

If the barrier is assumed to be of unit length in the y direction, then the total free energy of the barrier is (Lebwohl and Stephen, 1967):

$$F = \frac{\hbar j_1}{2e} \int dx [(1 - \cos\phi)] + 1/2 \lambda_0^2 \left(\frac{\partial\phi}{\partial x} \right)^2 + 1/2 \left(\frac{\lambda_0}{\bar{c}} \right)^2 \left(\frac{\partial\phi}{\partial t} \right)^2, \quad (3)$$

where the first term is the coupling energy for two superconductors and the others the electromagnetic energy in the barrier. The rate of dissipation of energy is:

$$dF/dt = -\sigma \int V^2 dx \quad (4)$$

We may note here, in anticipation of conclusions to follow, that removal of any terms in the left hand side of Equ. (3) will reduce energy dissipation.

Recognition of an analogy came about when Young (1964) pointed out that solutions of Equ. (2) representing vortex lines in the barrier are obtained as solutions of:

$$\partial^2\phi/\partial x^2 = (1/\lambda_0^2) \sin\phi, \quad (5)$$

which, except for sign, is the equation of a pendulum.

Next, the second model, the pendulum line, is considered as mechanical analog of the long Josephson junction. Figure 1 sketches a simple model with moment arm, I_c , moment of inertia, M , provided by a fly wheel, damping coefficient, D ,

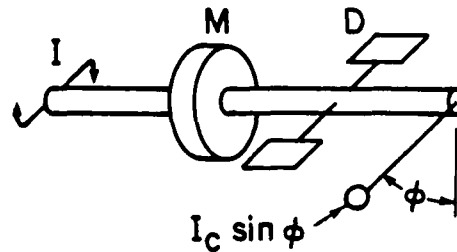


Fig. 1 After Fulton (1977).

provided by a paddle wheel arrangement, and phase angle ϕ measured from vertical downward. The rod is subject to an external torque I .

In the terms of such a model, one may list major corresponding quantities for Josephson circuits, the pendulum analog (Fulton, 1977) and trans polyacetylene:

TABLE I. After Fulton (1977) with extrapolation to polymer dynamics

<u>Josephson Junction</u>	<u>Symbol</u>	<u>Mechanical</u>	<u>(CH)_x</u>
Critical Current Maximum	I_c	Pendulum	u: charge dq_c/dt related to maximum pseudo spin vector by $\frac{dq_c}{dt} = \frac{\mu}{d\phi/dt}$ $= g_J \gamma J/d\phi/dt$ d: charge $e dq_c/dt$
Phase Difference	ϕ	Phase Angle Pendulum	u: π -phase kinking. d: π -phase kinking.
Voltages $\times 2\pi/\phi_0$	$d\phi/dt$	Angular Velocity	u: voltage $\times 2\pi/\phi_0$ related to spin angular momentum $\omega = 2\mu_B B/h$ by $d\phi/dt = \hbar\omega/(2m\phi_0 dq_c/dt)$. d: voltage $\times 2\pi/\phi_0$

TABLE I (Cont'd)

<u>Josephson Junction</u>	<u>Symbol</u>	<u>Mechanical</u>	<u>(CH)_x</u>
Applied Current	I	Applied Torque	u: applied current, dq/dt , related to the precessional radius of the spin vector by $dq/dt = \hbar\omega/(2m\phi \, d\phi/dt)$ d: applied ^o current, dq/dt .
$\phi_0/(2\pi R)$	D	Damping Coefficient	u: none for ideal system. d: $dq_d/dx = D$, dissipation to external phonon matrix.
$C\phi_0/(2\pi R)$	M	Moment of Inertia	u: dq_m/dx , charge repulsion. d: dq_m/dx , charge repulsion.
$\phi_0/(2\pi L)$	K	Torsion Bar Spring Constant	u: dq_K/dx , excitonic coupling. d: dq_K/dx , excitonic coupling.
Current in Inductor	I_L	Torsion in Torsion Bar	u: dq_L/dt determining phonon energy. d: dq_L/dt determining phonon energy.
Josephson Coupling Energy $-(\phi_0 I_c / (2\pi)) \cos\phi$		Gravitational Potential Energy $-I_c \cos\phi$	u: $-dq_c/dt \cos\phi$, exciton-phonon coupling energy. d: $-dq_c/dt \cos\phi$, exciton-phonon coupling energy.
Electrostatic Energy $1/2 CV^2$		Kinetic Energy $1/2 M(d\phi/dt)^2$	u: kinetic energy related to paramagnetic susceptibility by $\frac{1}{2} \frac{dq_M}{dx} \left(\frac{d\phi}{dt} \right)^2 =$ $\times \frac{\phi_0}{2\pi} \frac{d\phi}{dt}$ d: kinetic energy: $\frac{1}{2} \frac{dq_M}{dx} \left(\frac{d\phi}{dt} \right)^2$

TABLE I (Cont'd)

<u>Josephson Junction</u>	<u>Symbol</u>	<u>Mechanical</u>	<u>(CH)_x</u>
Magnetic Energy $1/2 LI_L^2$		Torsional Energy $1/2 I_L^2/K$	u: $1/2 (dq_L)^2/dq_K$, magn. $\frac{dt}{dx}$ energy d: $1/2 (dq_L)^2/dq_K$, magn. $\frac{dt}{dx}$ energy
Power Input from Applied Current IV		Power Input from Applied Torque, $dq/dt \cdot d\phi/dt$	u: $dq/dt \cdot d\phi/dt$, power input from applied field. d: $dq/dt \cdot d\phi/dt$, power input from applied field.

u = undoped polyacetylene;

d = doped polyacetylene;

$\phi_0 = h/2e = 2.068 \times 10^{-15}$ Webers;

and $Kd^2\phi/dx^2 = I_{c_x} \sin\phi + Dd\phi/dt + Md^2\phi/dt^2 + I_x$, or

$$\frac{dq_L}{dt} \frac{d\phi}{dt} = \frac{dq_c}{dt} \sin\phi + \frac{dq_D}{dx} \frac{d\phi}{dt} + \frac{dq_M}{dx} \frac{d^2\phi}{dt^2} + \frac{dq}{dt} \frac{d\phi}{dx},$$

and $d\phi dx = LI_L = (\phi_0/2\pi)d\phi dx$.

Some predictions can be made for the current-voltage relations of polyacetylene on the basis of this model. Firstly, in steady state there is an average current balance given by:

$$\langle I \rangle = \langle I_c \sin\phi \rangle + \langle V \rangle / R. \quad (6)$$

Decomposing I and V into steady and alternating components: $I = \langle I \rangle + \langle I_{ac} \rangle$ and $V = \langle V \rangle + \langle V_{ac} \rangle$, then if I is fixed $\langle I_c \sin\phi \rangle = \langle V_{ac}^2 \rangle / R$ and there should be a departure of the I-V curve from ohmic behavior, indicating that the voltage has an alternating component.

Secondly, if a radio frequency current at frequency, f, is applied near the junction frequency $\langle V \rangle / \phi_0$, the ac supercurrent locks into phase coherence with applied currents so that $\langle V \rangle = f$ giving linearity.

In order to obtain the characteristic particle in a double potential (Φ) well with harmonic spring connection to neighbor(s) (Figure 2),

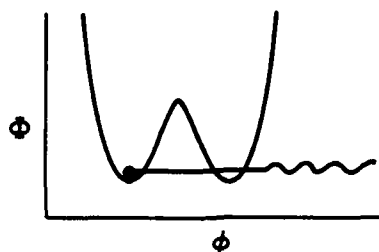


Fig. 2

an inductively connected element is required with phases: $\phi = 2\pi \int (V/\Phi_0) dt$ and $\theta = 2\pi \int (V_z/\Phi_0) dt$, where V and V_z are the voltages across the junction and an external passive element z , i.e., the next neighbor (Fulton, 1977):

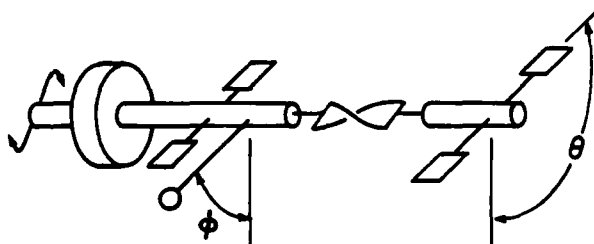


Fig. 3

Alternatively, the ϕ of Figure 2 is the angle of the carbon bond defining the isomerized state in $(CH)_x$, and the Φ is the configurational potential. Thus, the two potential well defines two isomerized states in polymers. If z , the external passive element is considered a resistor, r , ($z = r$), then for an undamped junction having $LI_c/\Phi \gg 1/2\pi$, there is the possibility of a relaxation oscillation if $L/r \gg (LC)^{1/2}$. If, on the other hand, z is the capacitor, C_z , and we define $C_{eff} = (1/C + 1/C_z)^{-1}$, then a resonance occurs at a frequency: $\omega_{res} = (LC_{eff})^{1/2}$, when the impedance of the C - L - C_z combination becomes infinite.

An inquiry may now be made concerning what happens when a polymer such as polyacetylene undergoes an order-disorder-order transition with displacement, or isomerized state transition, e.g., for one element (monomer):

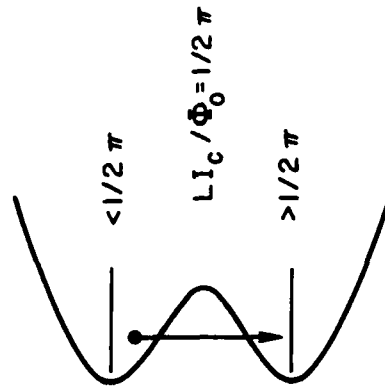


Fig. 4

For this situation of the monomer, z is an inductance, L , giving a T-bar twist, LI_c/Φ_0 , balancing the pendulum in a horizontal position. For $LI_c/\Phi_0 \ll 1/2\pi$, ϕ follows θ , but at $LI_c/\Phi_0 = 1/2\pi$ the pendulum is no longer stable and for $LI_c/\Phi_0 > 1/2\pi$ a flip to the other state occurs (Fulton, 1977):

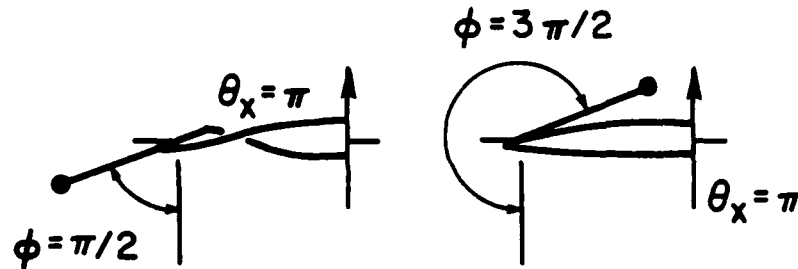


Fig. 5

Extrapolating this element to a one-dimensional chain analogous to the continuous limit of a dc SQUID, the equivalent circuit equation is:

$$K_\ell d^2\phi/dx^2 = I_{c\ell} \sin\phi + D_\ell d\phi/dt + M_\ell d^2\phi/dt^2 + I_{x\ell}. \quad (7)$$

where $I_{c\ell}$ is the critical current/unit length, $I_{x\ell}$ is the current/unit length applied to the junction, $K_\ell = \Phi_0 W/2\pi (2+d) = \Phi_0/2\pi L_\ell$, L_ℓ is the inductance/unit length, $M_\ell = \epsilon_0 \hbar W \Phi_0/2\pi d = \Phi_0 C_\ell/2\pi$, C_ℓ is the capacitance/unit length, $D_\ell = \sigma W \Phi_0/2\pi$, and σW is the conductance/unit length. We are especially interested in the behavior of this chain for $\ell \gg \lambda_J$, where $\lambda_J = (\Phi_0/(2\pi\mu_0(2\lambda+d)j_c))^{1/2}$, when vortex propagation is exhibited. Current propagation is described by:

$$K_{\ell} d^2 \phi / dx^2 = I_{c\ell} \sin \phi + I_x \ell, \quad (8)$$

which is in the same form as:

$$M d^2 \phi^1 / dt^2 = -I_c \sin \phi^1 + I_x, \quad (9)$$

describing the motion of an undamped pendulum subject to an external torque (see equation (5), above). A vortex (or propagating polymer soliton) in this analogy is as follows: a pendulum starts in a pendulum bob-down position (order) swings up (disorder) falls over through 2π and comes to rest in a pendulum bob-down position again (order). Conservation of kinetic and potential energy gives $1/2(d\phi/dx)^2 = (1-\cos\phi)\lambda_J^2$ for such motion, resulting in the description given by Figure 6. The two bob-down positions correspond to the two polymer isomerized states.

It is known that in a uniform pendulum array of infinite length, a full twist or vortex can be moved from place to place with no cost in energy (Scott, 1969; Waldram et al, 1970; Lebwohl and Stephen, 1967). Application of a weak torque in the vicinity of a vortex causes the pendulums to rotate in the direction of the applied torque and the twist moves along the array away from the torque. This is the propagating soliton of the displacive mode of the system. If two solitons are propagated along a pendulum array then in an overdamped system the two will be annihilated, in an underdamped system the two pass right through each other and continue on with their relative kinetic energies intact.

Consideration may now be given concerning how it is that the vortex, or π -phase-kink, becomes a propagating soliton. Stated differently, how does the order-disorder transition mode become a displacement transition mode? At the heart of the matter is the demonstration by Pitaevskii (1959), that for a system:

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} - \frac{\partial \Psi}{\partial t} (|\Psi|^2 - 1) \Psi = 0, \quad (10)$$

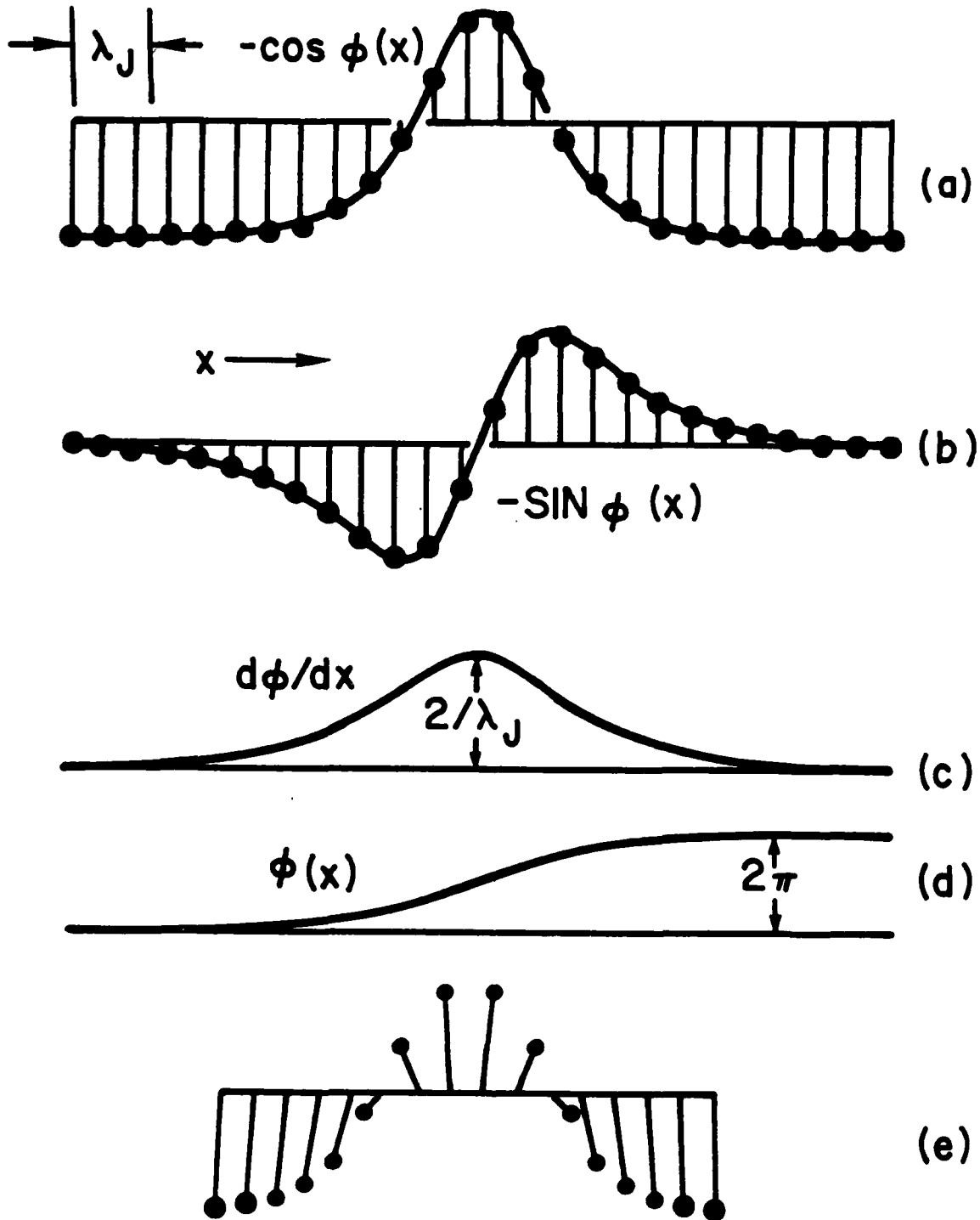


Fig. 6. Various views (a) to (d) of a segment of an infinitely long pendulum array containing a vortex. (a): Front view ($\cos \phi(x)$), (b): Top view ($-\sin \phi(x)$), (c): $d\phi/dx$, (d): $\phi(x)$. (e): A vortex trapped in an array of finite length by the excessive weight of the end pendulums. (From Fulton, 1977.)

the change of the complex function with time, t , is described by the equation: $i\hbar\partial\Psi/\partial t = \hat{L}$ where \hat{L} is a nonlinear operator and a function of a second variable - temperature in the system considered by Pitaevskii. As this second variable increases, the anti-Hermitian part of \hat{L} becomes dominant (as compared with the Hermitian). In this case, the equation which describes the vortex filament goes from Schrödinger type to diffusive type (Pitaevskii, 1959, 1961; Usui, 1969). In effect, the anti-Hermitian part of \hat{L} is larger, the faster the system relaxes. \hat{L} cannot be Hermitian for a propagating wave (soliton), because density would then be conserved and relation is required. If \hat{L} is Hermitian, then the wave is static (pinned).

The anti-Hermitian part describes the process whereby thermodynamic equilibrium is approached, or describes the process whereby the density of states and monomer 1 in a chain are converted into the density of states at the next monomer, monomer 2 (Barrett, 1983). A nonlinear operator gives:

$\partial E/\partial t + \text{div} Q = 0$, wave Q is an energy loss vector. For

"superconductivity" or decrementless conduction between monomers 1 and 2:

$$\text{div} Q_1 + \text{div} Q_2 = 0; \quad (10A)$$

$$\partial E_1/\partial t + \partial E_2/\partial t = 0. \quad (10B)$$

In the case of the anharmonic oscillator, we have $\partial\phi/\partial t = \hat{L}V$, or

$$\phi = \underbrace{\frac{C}{2} \frac{n \cdot n}{\ell \ell'}}_{\text{Hermitian Component}} + \underbrace{\frac{(\sum (X^2 + \frac{A}{B} x + C) + (u(\ell) - u(\ell'))^2)}{\ell}}_{\text{Anti-Hermitian Component}} \quad (10C)$$

where x is the position of, e.g., a carbon bond (for (CH_x)),

ϕ is configurational potential, and

ℓ is the length of the polymer.

In the case of the Davydov vibrational (protein) soliton, we have

$$\partial a/\partial t = \hat{L}a, \text{ or}$$

$$(i) \quad \frac{i\hbar da}{dt} = \frac{E_0 + W +}{\text{Hermitian Component}} \quad (10D)$$

$$+ X_1(\beta_{n+1,\alpha} - \beta_{n-1,\alpha}) a_{n\alpha} - J(a_{n-1,\alpha} + a_{n+1,\alpha}) +$$

$$+ L(a_{n,\alpha+1} + a_{n,\alpha-1}) +$$

$$+ \frac{X_2(\beta_{n+1,\alpha} a_{n+1,\alpha} - \beta_{n-1,\alpha} a_{n-1,\alpha} - \beta_{n\alpha}(a_{n+1,\alpha} - a_{n-1,\alpha}))}{\text{Anti-Hermitian Component}}$$

$$(ii) \quad \frac{\hbar d^2\beta}{dt^2} - W(\beta_{n+1,\alpha} - 2\beta_{n\alpha} + \beta_{n-1,\alpha}) \quad (10E)$$

$$\frac{\text{Hermitian Component}}{\text{Anti-Hermitian Component}}$$

$$= \frac{X_1(|a_{n+1}|^2 - |a_{n-1}|^2)}{\text{Anti-Hermitian Component}}$$

Anti-Hermitian Component

where X_1 and X_2 are nonlinear coupling coefficients,

J and L are dipole coupling coefficients,

$E_0 = 1650 \text{ cm}^{-1} = 0.205 \text{ e.v.}$,

a is the probability of finding a quantum of bond energy,

β is longitudinal displacement.

Thus, in considering whether a polymer can exhibit soliton behavior, neither the existence of isomerized states nor the existence of vibrational modes of energy compatible with an energy input is sufficient condition for propagating waves. Only if the anti-Hermitian component of the equation of state exceeds the Hermitian component will a perturbation become dispersive or propagate (Barrett, 1983).

Given that a polymer chain will support a soliton, consideration may be given as to whether a bifurcating chain (T-junction) will allow soliton propagation down the arms of the chain.

III. T-JUNCTIONS

Consider, then, three chain polymers joined at one end to form a T or Y junction. Such joined chains may be referred to as T junctions. In the Josephson line of one dimension Equ. (2), above, becomes (Scott, 1970):

$$K \frac{\partial^3 \phi}{\partial x^2 \partial t} + \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} - \Gamma \frac{\partial \phi}{\partial t} = \sin \phi - \gamma \quad (11)$$

where $K = L(2\pi J_c / \Phi C)^{1/2} / r$.

$$\Gamma = g(\Phi_0 / 2\pi J_c C)^{1/2},$$

$$\gamma = j_B / J_c$$

$$\Phi_0 = h/2e$$

J_c = a constant giving the maximum Josephson current per unit length:

L , C , r , g and j_B are the series inductance, the shunt

capacitance, the series resistance, the shunt conductance, the

distributed bias, and the current source per unit length, and

where distances are measured in units of $\tau_J = (\Phi_0 C / 2\pi J_c)^{1/2}$.

Simply stated K and Γ are losses in the line and γ represents bias.

In the case of pendula line T-junctions, Nakajima et al. (1976) define two classes: (1) the TTP (trigger turning point), which is analyzed by the two-dimensional equation reported by Nakajima et al. (1974a and 1978c). The boundary condition for the TTP is:

$$\phi_{x_1}|_{tp} = \phi_{x_2}|_{tp} = \phi_{x_3}|_{tp} \quad (12)$$

(2) A second turning point is the STP (selective turning point), with:

$$\phi_{x_1} + \phi_{x_2} + \phi_{x_3} = 0. \quad (13)$$

Thus, a single flux quantum propagating toward an STP on one line will initiate a single flux quantum on only one connected line, depending on the bias current of each line, the applied magnetic field and the junction geometry.

Confirming attention to the TTP junction and commencing with the two-dimensional description of Equ. (10), above: the motion of a vortex filament at temperatures close to the λ -point may be described. As the stability of a vortex is not guaranteed for a real field in two dimensions, Nakajima et al. (1978c) introduce a complex field:

$$\psi = \text{Re } \psi + i \text{Im } \psi \quad (14)$$

with now:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial t} \right) \text{Re } \psi = \frac{\partial U_R}{\partial \text{Re } \psi} \quad (15)$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial t} \right) \text{Im } \psi = \frac{\partial U_I}{\partial \text{Im } \psi} \quad (16)$$

where the potentials U_R and U_I are related by:

$$U_R = \frac{1}{4} (\text{Re } \psi)^4 - \frac{1}{2} [1 - (\text{Im } \psi)^2] (\text{Re } \psi)^2, \quad (17)$$

$$U_I = \frac{1}{4} (\text{Im } \psi)^4 - \frac{1}{2} [1 - (\text{Re } \psi)^2] (\text{Im } \psi)^2.$$

As the complex field possess a phase angle, clockwise and anti-clockwise vortices are obtained. With the condition stated by Equ. (12) satisfied, then, neuristor-like activities are possible (Crane (1962)) and describable in two-dimensional form (Equ. (10)) with a complex field.

The problem of defining specifications for propagation of solitons through (a) a TTP junction and (b) STP junction may be approached as follows: In the case of (a), the TTP junction, the requirement is given in Equ. (12). As $\phi(t) = (2\pi\Phi_0) \int_0^T V(u) du$, we require the voltage $\times 2\pi/\Phi_0$ to be the same on all 3 arms of the T junction. This reduces to the simple conclusion that all three arms must be of similar polymer material and of the same length.

Case (b), the STP junction, is more complex. Referring now to Equ. (11), for a set Γ , a soliton at a turning point may (1) halt, (2) propagate into arm 1, (3) propagate into arm 2, or (4) propagate into arm 3, depending upon the ratio of the bias currents: $\gamma_1:\gamma_2:\gamma_3$. γ corresponds to the applied torque, I , of the single junction (Table I). This, in turn, is a function of the amount of "pinning", i.e., introduction of defects into the polyacetylene, in order to obtain critical current increases at an appropriate applied field (Jaklevic et al. 1965, Yamashita et al. 1974). In order to predict which of the behaviors (1) - (4) will occur, one also needs an estimation of $d/2\lambda_J$, where $2\lambda_J$ is the length of the soliton and d is the

length of the polyacetylene (Owen and Scalapino, 1967). An easy conceptual solution is thus to uniformly dope a length of $(CH)_x$ (i.e., set $\gamma_1 = \gamma_2 = \gamma_3$) and synthesize T-junctions of different arm lengths for different $d_1 | 2\lambda_J : d_2 | 2\lambda_J : d_3 | 2\lambda_J :$

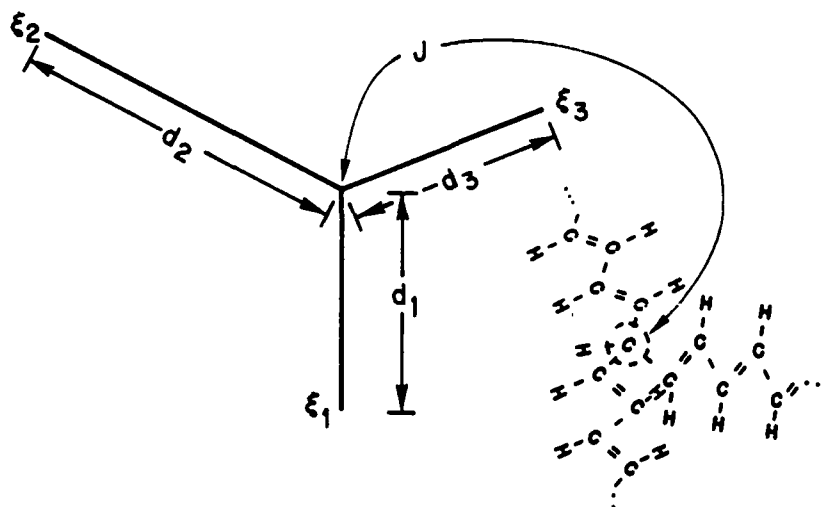


Fig. 7

In the vicinity of the junction J , the normal phonon modes will be different from those at the ends ξ_1 , ξ_2 and ξ_3 , or in the center of each chain. As soliton propagation of the moving charge domain-wall-type is dependent upon exciton-phonon coupling, the arrival of a soliton in the vicinity of J should show different propagating behavior compared with its behavior at a distance from the junction, due to different phonon-dependent propagation energies for that carbon atom at the T junction marked with a J (Fig. 7). This situation is different, therefore, from the pendulum line as the T junction in polymeric form exhibits different monomer vibrational forms at the T join; and the likelihood is that the soliton would not progress past the junction into arms d_2 and d_3 but be pinned there.

IV. TUNNELING

In the previous sections, treatment of soliton propagation in a one-dimensional organic conductor, trans-polyacetylene, was made in analogy with

fluxon propagation. This treatment is extended here to the case of uneven doping and unevenly conjugated conductors.

Parametric excitation is the underlying dynamic of the pendulum analogy as well as the Josephson effect.

We commence with Eq. (3) of section II for the total free energy for a Josephson barrier:

$$F = \frac{\hbar j_1}{2e} \int dx [(1 - \cos \phi) + \frac{1}{2} \lambda_0^2 \left(\frac{\partial \phi}{\partial x}\right)^2 + \frac{1}{2} \left(\frac{\lambda_0}{c}\right)^2 \left(\frac{\partial \phi}{\partial t}\right)^2], \quad (18)$$

in which the rate of energy dissipation is:

$$\phi' = (1 - \cos \phi) + \frac{1}{2} \lambda_0^2 \left(\frac{\partial \phi}{\partial x}\right)^2 + \frac{1}{2} \left(\frac{\lambda_0}{c}\right)^2 \left(\frac{\partial \phi}{\partial t}\right)^2. \quad (19)$$

Recalling that $\partial \phi / \partial t$ is the mechanical angular velocity or the Josephson junction voltage $\times 2\pi / \phi_0$, we now extend the voltage analogy to $\partial \phi / \partial x$ and call this term the dispersion voltage. As $(1 - \cos \phi)$ is the coupling energy, it is evident that Eq. (19) satisfies the condition for parametric excitation, where the $1/2 \left(\frac{\lambda_0}{c}\right)^2 \left(\frac{\partial \phi}{\partial t}\right)^2$ term is the pump, $(1 - \cos \phi)$ is the signal and $1/2 \lambda_0^2 \left(\frac{\partial \phi}{\partial x}\right)^2$ is the idler. Regarding a Josephson junction or polymer chain from a parametric excitation point of view permits the treatment of the line in discrete elements, dx . Variation of $d\phi/dt$ within any dx results in a variation of $d\phi/dx$, or dispersive transmission, due to the conservation condition of Eq. (19). The monomer for the polymer chain is described by the equation:

$$\phi' = f_0^3 + a f_0 + b = 0, \quad (20)$$

where f_0 may be taken as the midfrequency of a signal equivalent to electron momentum in the analysis of states. Eq. (20) is formally equivalent to Schrödinger's equation. If the following substitutions are made:

$$\begin{aligned}
 6uu_x &\rightarrow f_0^3, \\
 u_{xxx} &\rightarrow af_0, \\
 u_t &\rightarrow b,
 \end{aligned}
 \tag{21}$$

where subscripts indicate partial differentiation, then one has the Korteweg de Vries equation (Korteweg and de Vries, 1895):

$$u_t + 6uu_x + u_{xxx} = 0 \tag{22}$$

which is derived from the Boussinesq equation (Boussinesq, 1871):

$$u_{tt} = \frac{\partial}{\partial x} (u_x + 6uu_x + u_{xxx}), \tag{23}$$

by restricting the motion to one direction. We note that Eqs. (20) and (22) are formally similar.

If now, we consider a light wave polarizing energy levels of a polymer with, for example, two levels of energy, then the polarization may be decomposed into components in phase and in quadrature with the electromagnetic wave. The Schrödinger-type equation (20) for the atom reduces then to the Bloch equations for polarization or the self-induced transparency equations (Lamb, 1971). After transformation, these equations yield (Scott et al., 1973):

$$u_{xx} - u_{tt} = \sin u, \tag{24}$$

or the sine-Gordon equation.

The sine-Gordon equation is the unique equation invariant under the infinitesimal Lie transformation $x \rightarrow (1 - \epsilon)x$, $t \rightarrow (1 + \epsilon)t$ and the finite scale transformation $x \rightarrow a^{-1}x$, $t \rightarrow at$ and is Lorentz invariant (Bullough and Caudrey, 1980).

Now, the relations governing power flow in lossless nonlinear lumped circuit elements are the Manley-Rowe relations (Manley and Rowe, 1956). Considering the mean flux, N_u , of photons of frequency u , the analogous relations for extended lossless nonlinear media are (McLean, 1977):

$$N_{u1} + N_{u2} + N_{u3} = \text{constant}, \quad (25)$$

and

$$u_1 + u_2 = u_3. \quad (26)$$

Substituting:

$$\begin{aligned} u_{xx} &\rightarrow u_1, \\ u_{tt} &\rightarrow u_2, \\ \sin u &\rightarrow u_3, \end{aligned} \quad (27)$$

provides a formal similarity between the sine-Gordon eq. (24) and the equation describing parametric amplification (Eq. (26)). The relation of the sine-Gordon equation to electron tunnelling and the Josephson effect is already known (Bullough, 1977), by which the parallelism is drawn between the "kink" and "anti-kink" solutions of the sine-Gordon equation and the fluxons in large area Josephson junctions. Here, we point out the parallels between: (1) the Schrödinger formalism and the Korteweg-de Vries equation and (2) the sine-Gordon equation and the Manley-Rowe conservation equations.

We now utilize this development. Suppose the wave function for an electron, ψ , is given as a function of distance, x , the Schrödinger equation for which is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E, \quad (28)$$

where $V(x)$ is the amplitude of a barrier to free movement of the electron.

If V varies relatively slowly with distance, then the solution of Eq. (28) is (Messiah, 1958):

$$\begin{aligned} \psi &= \psi_0 \exp\left[\pm i \frac{2m}{\hbar} \sqrt{E - V(x)} x\right] \\ &= \psi_0 \exp[\pm i(\sqrt{u_{\text{idler}}})x] \\ &= \psi_0 \exp[\pm i(\sqrt{(u_{\text{pump}} - u_{\text{signal}})})x]. \end{aligned} \quad (29)$$

Adapting Eq. (26) to explicit parametric amplification form, we have:

$$u_{\text{pump}} = u_{\text{signal}} + u_{\text{idler}}. \quad (30)$$

Eqs. (29) and (30) are then interpreted as follows: $\frac{2m}{\hbar^2} E$ and $\frac{2m}{\hbar^2} V(x)$ are the spatial frequencies of two oscillating systems, Eq. (29) represents the situation of parametric excitation in which $\frac{2m}{\hbar^2} E = u_{\text{pump}}$ is the spatial frequency of the pump, $\frac{2m}{\hbar^2} V(x) = u_{\text{signal}}$ is the spatial frequency of the signal, and $\frac{2m}{\hbar^2} (E - V(x)) = u_{\text{idler}}$ is the spatial frequency of the idler. As (i), by definition, $V(x)$ is maximum at a different position, x , than is ψ i.e., it is a barrier, and as (ii) it is the pumped signal system which is of energy $V(x)$, it follows that a pumped idler system of spatial frequency $\frac{2m}{\hbar^2} (E - V(x))$ should appear at a distance x , i.e., out of the barrier. Whereas Josephson (1962) treated the term in the Hamiltonian which transfers electrons across the barrier as a perturbation, here we specifically designate it as a pumping system. Electron tunnelling is thus dispersive parametric excitation and may be given a classical mechanics point of view.

For example, the master equation for the effect is:

$$V_{\text{barrier}} = \psi(x)_{\text{in}}^2 - \psi(x)_{\text{out}}^2. \quad (31)$$

In the case of two superconductors connected by a 'weak link', the Josephson equations (Josephson, 1962, 1964, 1974) give:

$$j = j_0 \sin(\phi_2 - \phi_1 - \frac{2e}{\hbar} \int_1^2 A dx),$$

$$\frac{\partial}{\partial t} (\phi_2 - \phi_1 - \frac{2e}{\hbar} \int_1^2 A dx) = -\frac{1}{\hbar} (\mu_1 - \mu_2) = \frac{2eV}{\hbar}, \quad (32)$$

for a one-dimensional junction, and where j is the supercurrent through the junction, ϕ is the phase of the order parameter, A is the magnetic vector potential, μ is the chemical potential, and V is the voltage bias across the junction. Again, the junction bias acts as a signal to the second system as pump and the third as idler.

This is apparent in Josephson's (1964) account of the tunnelling effect. As the barrier is changed from a very thick one to a vanishingly

thin one, the system loses the degree of freedom corresponding to the ability to alter phases independently. The free energy of the system contains a contribution from the barrier region which depends on the relative phases of the values of ψ on the two sides of the barrier, and whose magnitude becomes greater as the barrier is made thinner. Perfect conductivity of a superconductor is the consequence of the fact that in a steady-state the order parameter must have the form (Josephson, 1964):

$$\Psi(r, t) = \Psi(r, 0) \exp [i \alpha(t)]. \quad (33)$$

Ψ will still have this form in a system partitioned by a barrier, provided that the phases of the order parameters on each side of the barrier are locked together by the barrier energy. The only way this can occur is by parametric excitation.

V. EFFECT OF PINNING

In sections I - III mention was made of the effect of removal of pendula for a length larger than $2\lambda_J$, where λ_J is the Josephson penetration length or $(K_0/mgl)^{1/2}$ in the model (K_0 is the twisting constant of the elastic coupling per unit length, l is the pendulum length, mg is gravitation), resulting in the pinning effect of a Josephson junction. Referring to Eq. (19) above, the effect of pinning results in the neglect of the $(1-\cos\theta)$ term, i.e., $\theta \rightarrow 0$. This term is the signal term of the parametric excitation dynamic, hence there can be no conduction beyond such a barrier. Conduction between barriers along a line of intact pendula is, however, possible. Such a segment would exhibit the properties of a soliton if short time constants are considered, and a trapped polaron if a long time constant is considered.

Pinning may be obtained in another way. The Josephson penetration length is a function of mg , hence weighting the pendula bobs would obtain

the same effect as removal of pendula. A pinned soliton (kink) is shown below:

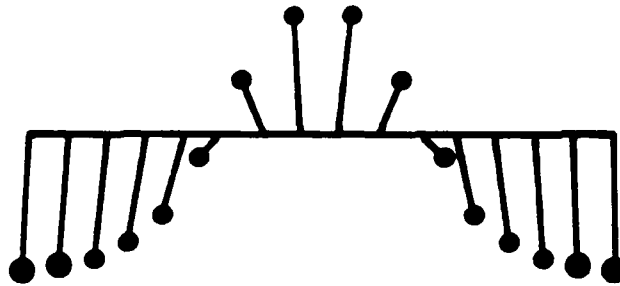


Fig. 8

The result of pinning (or doping) is firstly to provide a barrier to conduction. However, the critical Josephson current increases at an appropriate applied field. From the mechanical point of view this means that a torque is placed on the first pendulum of a magnitude such that either (a) the barrier of the vacated pendulum is traversed, or (b) the heavy bob of the second pendulum is raised. Either way, an angle θ is created for the second pendulum permitting a signal term $(1-\cos\theta)$ for parametric excitation.

The effect of nonuniform doping in, for example, $(CH)_x$, may be considered, i.e., when pendula are removed so that irregular spacings are created, or when the pendula have bobs of varying weight. These variations all result in variations in the θ s created at each dx along the chain. This, in turn, results in variations in the $(1-\cos\theta)$ or signal term at each dx . The conservation condition of parametric excitation then requires that increased doping, resulting in a smaller θ and hence a smaller signal term, gives a larger idler voltage. In short, increased doping should result in a larger voltage along the line due to increased resistance at constant current. Turned around, at constant voltage increased doping results in increased resistance hence decreased current. Simply stated, the tolerance

of an irregularly doped trans-polyacetylene chain is that of a line with resistances of various values in series.

Considering the problem from a more basic point of view, Eq. (20) above, is of the same form as:

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} - \frac{\partial \Psi}{\partial t} = (|\Psi|^2 - 1)\Psi, \quad (34)$$

which is Eq. (10) of section II. There, the demonstration by Pitaevskii (1959) was mentioned that for a system such as this, the change of a complex function Ψ with time is described by the equation: $i\hbar \partial \Psi / \partial t = \hat{L} \Psi$, where \hat{L} is a nonlinear operator. As the second variable increases, the anti-Hermitian part of \hat{L} becomes dominant (as compared with the Hermitian). In such an event, the equation which describes the polymer chain goes from Schrödinger type to diffusive type (Pitaevskii, 1959, 1961; Usui, 1969). Thus, the effect of an increase in doping, beyond a certain level discussed below, is an increase in Schrödinger type behavior, the effect of a decrease in doping, below this level, is to increase again diffusive type behavior. For a room temperature type conductor which is uniformly and ideally doped, we could obtain the same effect over time of nonuniform doping by a temperature fluctuation which resulted in a variation in the ratio of Schrödinger and diffusive type behavior. When there is behavior described only by a Schrödinger type equation, there may be a trapped polaron, but there is no conduction beyond the length considered.

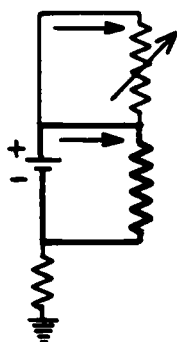
VI. OHM'S AND KIRCHOFF'S LAWS

In recapitulation: in a polymer chain of monomer length, dx , there can be either order-disorder Schrödinger type behavior or displacive behavior. In an electrically conducting polymer, the former behavior results in resistance, the latter, in conductance. These two modes can be related to the conservation laws: Ohm's law and Kirchoff's law.

Halperin, Hohenberg and Ma (1974, 1976) and Hohenberg and Halperin (1977) have studied the effects of different conservations on the energy and space integral of the order parameter. The order parameter in $(CH)_x$ is ϕ or the pseudo spin (undoped case) or bound charge (doped case), which can exchange energy with a reservoir that has either an infinite specific heat or an infinite thermal conductivity. The first case typifies resistance conduction and the second, decrementless conduction. Energy conservation can be achieved by choosing the damping constant Γ_0 appropriately. Four cases are then distinguished: (a) ϕ not conserved, E not conserved, and Γ_0 is a constant; (b) ϕ conserved, E not conserved, $\Gamma_0 = -\lambda_0 \nabla$; (c) ϕ not conserved, E conserved, Γ_0 is a constant; (d) ϕ conserved, E conserved, $\Gamma_0 = -\lambda_0 \nabla$. In terms of the mechanical analog, conservation of the pseudo spin corresponds to conservation of ϕ : conservation of energy corresponds to conservation of the applied torque; the constant Γ_0 corresponds to the damping coefficient D and moment of inertia M of Table I in section I; thus, $\Gamma_0 = -\lambda_0 \nabla$ indicates a known variation in the size and weight of pendula bobs.

In the analogy drawn, conservation of ϕ will occur only if Kirchoff's law applies to the system as an adiabatic system. Furthermore, Ohm's law entails conservation of energy in the system considered adiabatic. The four cases, A-D may thus be represented in terms of four nonadiabatic circuits (heavy lines) joined to reservoir circuits in series (lighter lines). The elements of the circuits consist of a battery, resistances and lead to ground:

A.



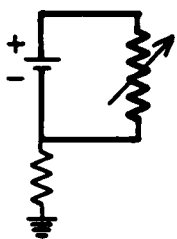
Mechanical

1. T junction coupling to other pendulum line.
2. T junction coupling to other elastic torque line.
3. Pendula bob weights on original line equal.

Trans (CH)_x

1. T junction coupling to other fibers unequally doped.
2. T junction coupling to other fibers of unequal excitonic coupling.
3. Original fiber uniformly doped.

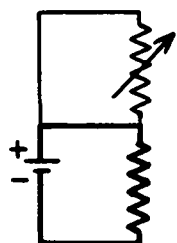
B.



1. No T junction to other pendulum line.
2. T junction to line offering elastic torque only.
3. Pendula bob weights on original line unequal.

1. No T junction
2. T junction to ligand offering different excitonic interaction from original fiber.
3. Original fiber non-uniformly doped.

C.



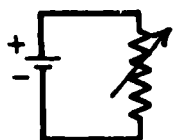
Mechanical

1. T junction coupling to other pendulum line.
2. No T junction to line offering elastic torque.
3. Pendula bob weights on original line equal.

Trans (CH)_x

1. T junction coupling to fibers unequally doped.
2. No T junction to fibers offering excitonic coupling.
3. Original fiber uniformly doped.

D.



1. No T junction to other pendulum line.
2. No T junction to other pendulum line.
3. Pendulum bob weights on original line unequal.

1. No T junction
2. No T junction
3. Original fiber nonuniformly doped.

Fig. 9

This description of trans-polyacetylene only applies to the displacive mode. This may be defined more accurately by consideration of the following classical Hamiltonian:

$$H = \sum_i \left(\frac{p_i^2}{2M_0} + \frac{1}{2} r_0 \psi_i^2 + U_0 \psi_i^4 \right) + \frac{1}{4} \sum_{ij} J_{ij} (\psi_i - \psi_j)^2, \quad (35)$$

where the subscripts i and j refer to points on a d -dimensional, simple cubic lattice with lattice constant unity, ψ_i is a scalar quantity describing the displacement of an atom in the i th unit cell, and $p_i = M_0 d\psi_i/dt$ is the momentum conjugate to ψ_i . The first term is of the same form as Eqs. (20) and (34) above. If $|r_0|/J_0 \gg 1$ the transition undergone by the system is an order-disorder (Schrödinger-like) transition: if $|r_0|/J_0 \gg 1$, the system undergoes a displacive transition (Hohenberg and Halperin, 1977). The above description for A, B, C, and D refers to the displacive transition only.

VII. DYNAMIC FORM FACTOR

Conducting trans-polyacetylene, proteins and DNA with soliton excitation are in the displacive transition mode, which exhibits unique attributes. The critical dynamics of such a phase transition is dominated by: (1) a soft phonon whose frequency decreases as the transition temperature is approached, and (2) the appearance of a central component around $\omega=0$ in the dynamic form factor (Schneider and Stoll, 1973, 1976, 1978, 1981). This dynamic form factor or spectral density is related to, and defined by, the characteristic frequency or relaxation time of a mode:

$$\frac{1}{\tau_{AA}(k)} = \tau_{AA}(k) = \hat{S}_{AA}(k, \omega=0) = 2 \int_0^\infty \frac{S_{AA}(k, t) dt}{S_{AA}(k, t=0)}, \quad (36)$$

where the correlation functions are (Schneider and Stoll, 1976):

$$\hat{S}_{AA}(k, t) = \frac{1}{S_{AA}(k, t=0)} S_{AA}(k, t), \quad S_{AA}(k, t) = \langle A(-k, 0) A(k, t) \rangle, \quad (37)$$

and related to the spectra densities or dynamic form factor by:

$$\hat{S}_{AA}(k, \omega) = \frac{2}{S_{AA}(k, t=0)} \int_0^{\infty} \frac{\sin \omega t}{\omega} S_{AA}(k, t) dt. \quad (38)$$

At the present time there is no firmly based analytical technique to calculate the quantities (36), (37) and (38) for a system evolving according to Newton's equations (Schneider and Stoll, 1981). These quantities are, however, of crucial importance in understanding the excitation spectrum. Schneider and Stoll (1973) reported that during the temporal development of this system clusters form, representing connected cells whose instantaneous local order parameter has a sign opposite to that expected. These propagating clusters in two or three dimensions are the equivalent of soliton propagation in the one-dimensional trans-polyacetylene. For small wave vectors where the frequency of the cluster waves is small, the damped cluster waves become overdamped and give rise to the central peak phenomenon. The central peak half-width is proportional to the inverse lifetime of the cluster waves and its height is proportional to this lifetime (Schneider and Stoll, 1976). The behavior of these clusters is consistent with the universality hypothesis for structural phase transitions. The prediction may be made, then, that (a) neutron scattering will detect a central component at $w=0$ in the dynamic form factor in the case of polymers excited to soliton propagation; and (b) that the dynamics of such polymers obey the universality hypothesis, if soliton propagation occurs.

This development can be placed in the context of the thrust of sections I-III. Iwamatsu and Onodera (1977) have derived an exact expression for the dynamical structure factor within the framework of classical statistical mechanics. These investigators commence with an equation analogous to Eq. (20):

$$H = \frac{M}{2} \dot{x}^2 + Ax^4 + Bx^2, \quad (39)$$

where M is the mass of the oscillator, x is the displacement of the oscillator from the origin or normal coordinate of a particular mode, B represents the coefficient of harmonic restoring force and A represents the contribution of anharmonicity. The anharmonic potential $V(x) = Ax^4 + Bx^2$ has one or two minima depending on the sign of B :

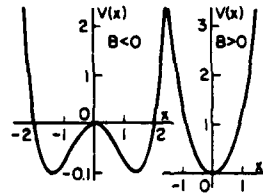


Fig. 10

However, the results obtained can be generalized to a nonlinear oscillator moving in a quite general potential (Matsubara, 1972), for example:

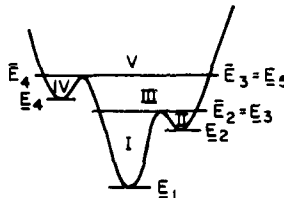


Fig. 11

An equivalence between Eq. (39) and Eq. (20) is obtained for: $a=B/A$, $b=M\dot{x}^2/2A$, $B=aA$, and the energy E is in units of $B^2/4A = a^2A/4$. In the case of $E < 0$ ($B < 0$) the motion of the oscillator is confined within one of two wells and the solution is the Jacobian elliptic function (Onodera, 1970):

$$x(t) = a \operatorname{dn}(\Omega_0 t - \operatorname{dn}^{-1}(x/a)) \quad (40)$$

where $\Omega_0 = (1+E)^{1/4}$. The fundamental frequency of oscillation is:

$$\Omega(E) = \frac{2\pi\Omega_0}{2K(k)} = \frac{\pi}{K(k)} \frac{(1+1+E)^{1/2}}{2} \quad (41)$$

where $K(k)$ is the complete elliptic integral of the first kind. The dependence of $\Omega(E)$ on the energy E is (Iwamatsu and Onodera, 1977):

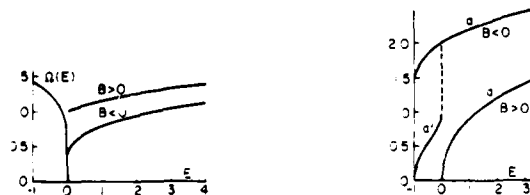


Fig. 12

The degree of anharmonicity is given by the modulus k :

$$k^2 = 1/2 (1 - \frac{\text{sgn} B}{\sqrt{1+E}}), \quad B > 0, \quad (42a)$$

$$k^2 = \frac{2}{1 + (1+E)^{-1/2}} \quad B < 0, \quad (42b)$$

and the amplitude of harmonic oscillation and anharmonic oscillation is:

$$a^2 = 2(\sqrt{1+E} - \text{sgn} B), \quad B > 0, \quad (43a)$$

$$a^2 = 2(1 + \sqrt{1+E}), \quad B < 0, \quad (43b)$$

$$a^1 = \frac{a}{2} (1 - \sqrt{1-k^2}). \quad (43c)$$

The oscillation amplitude versus energy for two wells is:

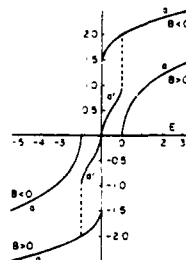


Fig. 13

The dynamic structure factor $S(k, \omega)$ is:

$$S(k, \omega) = S_1(k, \omega)/Z, \quad \text{for single-minimum potential case} \quad (44a)$$

$$S(k, \omega) = \frac{S_1(k, \omega) + 2S_2(k, \omega)}{Z_1 + 2Z_2} \quad \text{for the double-minimum potential case} \quad (44b)$$

$$\text{where } Z_1 = \int_0^\infty dE e^{-E/T} / \Omega(E),$$

$$S_1(k, \omega) = \int_0^\infty dE e^{-E/T} \sum_{n=-\infty}^{\infty} |\alpha_{1n}(k, E)|^2 \frac{1}{\Omega(E)} \delta(\omega - n\Omega(E)),$$

$\alpha_{1n}(k, E)$ is the Fourier coefficient of the periodic function $\exp(ikacn\Omega_0 t)$

or

$$\alpha_{1n}(k, E) = \frac{1}{T(E)} \int_0^{T(E)} e^{ikacn\Omega_0 t} e^{-in\Omega(E)t} dt,$$

$$S_2(k, \omega) = \int_{-1}^0 dE e^{-E/T} \sum_{n=-\infty}^{\infty} |\alpha_{2n}(k, E)|^2 \frac{1}{\Omega(E)} \delta(\omega - n\Omega(E)),$$

$$Z_2 = \int_{-1}^0 dE e^{-E/T} \frac{1}{\Omega(E)}, \quad \text{and}$$

$\alpha_{2n}(k, E)$ is the Fourier coefficient of the periodic function $\exp(ikadn\Omega_0 t)$

or

$$\alpha_{2n}(k, E) = \frac{1}{T(E)} \int_0^{T(E)} e^{ikadn\Omega_0 t} e^{-in\Omega(E)t} dt.$$

It follows from these expressions that $|\alpha_{1n}|$ and $|\alpha_{2n}|$ have local maxima when the transferred wavelength $\lambda=2\pi/k$ or its positive integer multiples, is nearly equal to the oscillation amplitude, i.e., when:

$$ka \text{ or } ka^{\frac{1}{2}} \sim \frac{\pi}{2} (2p-1), (p=1,2,\dots). \quad (45)$$

This means that particular oscillations that have a oscillation amplitude comparable with the transferred (transmitted) wavelength (or positive multiples thereof) may resonate with a perturbation offered by a neutron beam, i.e., inelastic neutron scattering is a possible investigative tool. This has, indeed, been demonstrated for SrTiO_3 , KMnF_3 and KTaO_3 (Shirane, 1974). The expectation is that trans-polyacetylene will demonstrate similar scattering.

The dynamic structural phase transition accompanied by the softening (i.e., by acting as pump) of a particular mode of lattice vibrations is shown in the following example (Iwamatsu and Onodera, 1977):

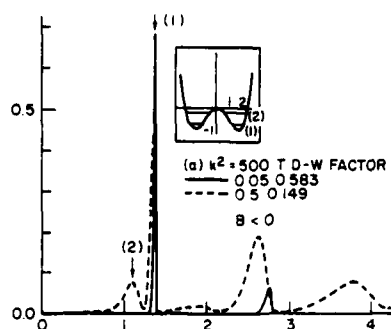


Fig. 14

This constitutes the strongest piece of evidence that soliton propagation for the $(\text{CH})_x$ type of polymers is pumped by a phonon mode with phonon-exciton coupling as stated above.

The question of tolerance in soliton propagation in an irregularly doped transpolyacetylene line thus may be translated into a calculation of the dynamic form factor for a particular nonlinear oscillator moving in a general potential at a particular dx on the line.

VIII. NECESSARY AND SUFFICIENT CONDITIONS FOR SOLITON PROPAGATION

One may ask what is so special about organic conductors? Other systems undergo phase transitions. The answer is that those which do not conduct, do not, at the critical temperature, become displacive. From the point of view of that most basic of theories: fluctuation-dissipation theory, a simple answer is that when the vibrational wave vector becomes larger than the correlation length, displacement occurs. It is as if the vibrational cup runneth over (to become a pump for excitonic coupling). For $(CH)_x$ type of polymers, this can only occur when the energy of the normal mode of the vibrational levels within the electronic potential well becomes a magnitude that phonon-excitonic lateral coupling is possible. Parametric excitation then results, which is describable after translation, by Eqs. (19) and (24). The vibrational normal mode acts as a pump to the exciton as signal and the vibrational normal mode of the neighboring well as idler. In the pendulum analogy, the vibrational energy levels correspond to applied torque, in the long Josephson junction, to the applied current. The excitonic coupling corresponds in the pendulum analogy to the torsion-bar spring constant, and in the long Josephson junction to $\phi_0/2\pi L$. The analysis of the previous section thus extends the pendulum analogy to a consideration of the resultant effect of vibrational fluctuations in the applied torque.

The dynamics of fluctuations in a critical region is dominated by the role played by exchange of energy between the different hydrodynamic (long-wavelength) motions and the thermal reservoir (short-wavelength motions). For a small deviation from equilibrium, the rate of change of ϕ is proportional to:

$$\frac{\partial \phi}{\partial t} = - \frac{\Gamma \partial F}{\partial \phi}, \quad (46)$$

where Γ is a kinetic coefficient. As before, the ordering field is of the form:

$$F = \int \left[\frac{1}{2} a \phi^2 + \frac{1}{4} \lambda \phi^4 + \frac{1}{2} C (\vec{\nabla} \phi)^2 - h \phi \right] d^n x, \quad (47)$$

and thus the equation of motion (46) has the form with $c=1$ and $a=\tau$

(Patashinskii and Pokrovskii, 1979; Eilenberger, 1981):

$$\frac{1}{\Gamma} \frac{\partial \phi}{\partial t} - \nabla^2 \phi + \tau \phi + \lambda \phi^3 = h \quad (48)$$

Eq. (48) describes the situation depicted in Fig. 9D of section VI for which ϕ is conserved, E is conserved and $\Gamma_0 = -\lambda \nabla$.

For the case of A (ϕ and E are not conserved and Γ_0 is a constant), Eq. (46) is:

$$\frac{1}{\Gamma_0} \frac{\partial \phi}{\partial t} = - (\tau_0 \phi - \nabla^2 \phi + 4g_0 \phi^3) + h \quad (49)$$

For the case of B (ϕ is conserved, E is not conserved and $\Gamma_0 = -\lambda \nabla$), Eq. (46) is:

$$\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0, \quad (50)$$

where the flux \vec{j} is defined: $\vec{j} = \Gamma_0 \vec{\nabla} \langle f_{\text{ext}} - (\delta H / \delta \phi) \rangle$ and $f_{\text{ext}}(\mathbf{x}, t)$ is force externally applied.

For the case C (ϕ is not conserved, E is conserved and Γ_0 is a constant), Eq. (47) is (Patashinskii and Pokrovskii, 1979):

$$H = \int \left[\frac{1}{2} \tau_0 \phi^2 + \frac{1}{2} (\vec{\nabla} \phi)^2 + g_0 \phi^4 + \gamma_0 \varepsilon \phi^2 + \frac{1}{2} c_0^{-1} \varepsilon^2 \right] d^n x, \quad (51)$$

where two independent fields ϕ and ε are postulated obeying:

$$\frac{\partial \phi}{\partial t} = - \Gamma_0 \frac{\delta H}{\delta \phi} + h(\vec{x}, t), \quad (52a)$$

$$\frac{\partial \varepsilon}{\partial t} = - \Delta_0 \nabla^2 \frac{\delta H}{\delta \varepsilon} + \tau(\vec{x}, t). \quad (52b)$$

The case generalized to two fields ϕ_1 and ϕ_2 , where ϕ_1 is an m -component field and ϕ_2 is an n -component field is:

$$H = \int d^n x \left[\frac{1}{2} (\tau_1 \phi_1^2 + \tau_2 \phi_2^2) + \frac{1}{2} (\vec{\nabla} \phi_1)^2 + \frac{1}{2} (\vec{\nabla} \phi_2)^2 + g_1 (\phi_1^2)^2 + g_2 (\phi_2^2)^2 + g_{12} \phi_1^2 \phi_2^2 \right]. \quad (53)$$

Such a system has two phase transitions for which the renormalization group equations in four space are (Patashinskii and Pokrovskii, 1979):

$$\begin{aligned}\frac{dg_1}{d\xi} &= -4(m+8)g_1^2 - ng_{12}^2, \\ \frac{dg_2}{d\xi} &= -4(n+8)g_2^2 - mg_{12}^2, \\ \frac{dg_{12}}{d\xi} &= -4g_{12}((m+2)g_1 + (n+2)g_2) - 8g_{12}^2.\end{aligned}\quad (54)$$

This analysis also gives a relation to the susceptibility. Returning to Eqs. (46) and (47), we obtain the form:

$$\dot{\phi} = -\Gamma(a\phi + b\phi^3 - c\nabla^2\phi - h). \quad (55)$$

If ϕ is close to the equilibrium value ϕ_0 , this equation can be linearized ($\phi = \phi_0 + \delta\phi$):

$$\frac{1}{\Gamma} \dot{\delta\phi} - c\nabla^2\delta\phi + \frac{\delta\phi}{\chi} = 0. \quad (56)$$

Changing to the Fourier components:

$$\delta\phi(\vec{q}) = \int \delta\phi(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} d\vec{x}, \quad (57)$$

We see that their relaxation time depends on q :

$$t_c^{-1}(q) = \Gamma/\chi(q). \quad (58)$$

and the susceptibility for a given q is determined by the relation (Patashinskii and Pokrovskii, 1979):

$$\chi^{-1}(q) = \chi^{-1}(0) + cq^2. \quad (59)$$

Could, then, any arbitrary polymer system exhibit soliton propagation? Only if it has the requisite hydrodynamic vibrational and relaxational modes which occurs when the wavenumber, q , and frequencies, ω , of the hydrodynamic vibrational and relaxational motions are:

$$\begin{aligned}q &\ll 1/r_c, \\ \omega &\gg 1/t_c,\end{aligned}\quad (60)$$

where r_c is the static correlation length and t_c is the relaxation time.

If, then, we divide a trans-polyacetylene chain into cells Ω_{dx} with linear dimensions $dx \ll r_c$, and stipulate that in each of these cells the total

order parameter varies with time, the characteristic time $t(dx)$ has a well defined scaling dimension dt :

$$t(dx) \sim dx^{-dt}, \quad (61a)$$

and the inverse $\omega(dx) = t^{-1}(dx)$ is the characteristic frequency of a fluctuation of size dx (i.e. of the size of one monomer of $(CH)_x$). For a $q \gg 1/r_c$ i.e., not the hydrodynamic but the fluctuational mode, the dispersion of the fluctuational mode is:

$$\omega \sim q^{-dt} \quad (61b)$$

Location of the hydrodynamic (both vibrational and relaxational modes) and the fluctuational mode is shown below (after Patashinskii and Pokrovskii, 1979):

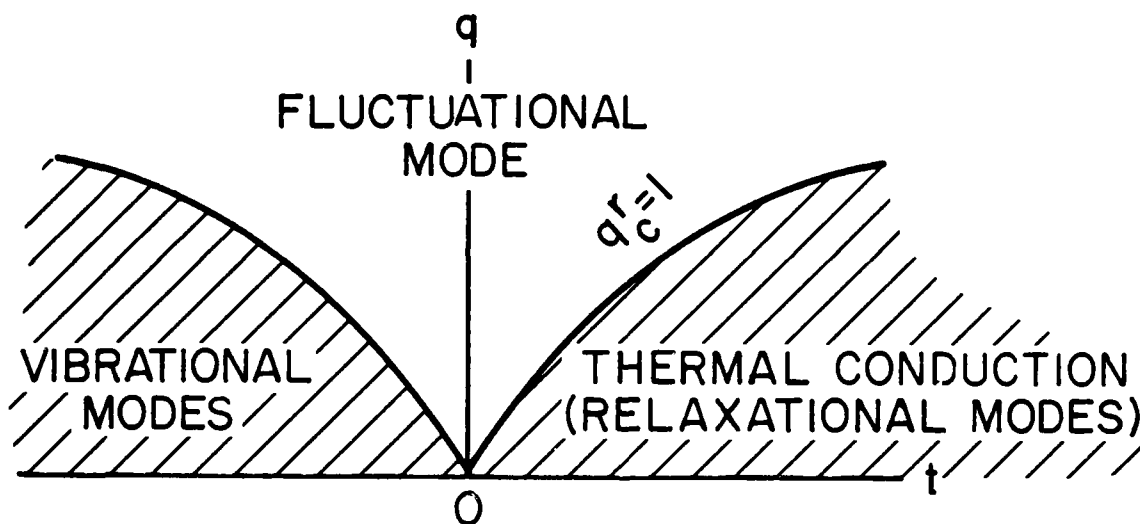


Fig. 15

The hydrodynamic modes, the vibrational and relaxational, are associated with the transport of additive conserved quantities such as spin and electric charge. In the case of the vibrational mode, there is almost no dissipation, so case D above, belongs to this category as does a single line of trans-polyacetylene. In the case of the relaxational mode fluxes are proportional to the gradients of hydrodynamic quantities, and cases A, B, and C above, belong to this category.

IX. CHANGING AND INCOMPLETE DEGENERACY

a. Introduction

Trans-polyacetylene, $(CH)_x$, is electrically conducting and the underlying mechanism mediating this conduction is thought to be due to the presence of dynamic force relations describable by the mathematical entity of the soliton (Heeger and MacDiarmid, 1981). There are a number of current-voltage relations reported for $(CH)_x$ which show a quadratic dependence of current on the voltage (Shirakawa et al., 1978; Park et al., 1980; Epstein et al., 1980; Roland et al., 1980; Gould et al., 1981; Moses et al., 1981; Chiang and Franklin, 1981; Yamamoto et al., 1980) (cf. Figure 1). With the dopant concentration $y > 10^{-2}$ the EPR signal is significantly reduced from that of the undoped (and electrically nonconducting) trans- $(CH)_x$; and for $y > 2 \times 10^{-2}$ the signal vanishes (Ikehata et al., 1980; Chien et al., 1982), indicating that the dopant binds to free electrons providing the conditions for electron-free, charged excitation (soliton) propagation. This doping is, however, not expected to be uniform throughout any $(CH)_x$ chain.

There have been a considerable number of theoretical treatments of soliton propagation in $(CH)_x$ (Su et al., 1979, 1980; Kivelson, 1981a,b). A different point of view is considered here permitted by the NMR observations of Nechtschein et al (1980) on changes in the proton relaxation rate upon doping of $(CH)_x$ and by Chen et al., (1978) that doping adds to the double bond and at the highest concentration results in the formation of a substituted polyethylene. These observations suggest that the doping process results in a competition between the dopant and the hydrogen (state of resonance) for a carbon bond.

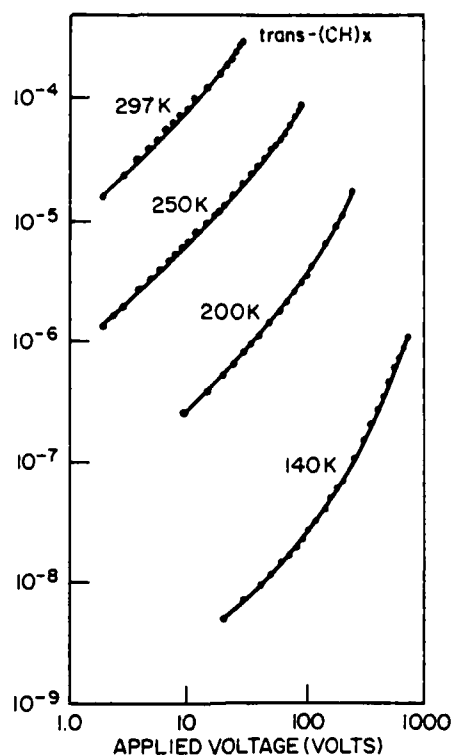


Fig. 16. Current-voltage characteristics of trans-(CH)_x at various temperatures. From (Yamamoto et al., 1980).

As electrical conductivity in (CH)_x is dependent upon this doping, considered nonuniform, the possible reasons are examined here for the quadratic current-voltage relations in trans-(CH)_x using a soliton charge carrying mechanism based on the anharmonic oscillator model (Chen et al., 1978).

b. Anharmonic Oscillator Model

The anharmonic oscillator model is based on the equation of motion for a monomer of the general form (Bruce, 1978; Bruce and Cowley, 1980):

$$\ddot{\phi} = -x^2 + \frac{A}{B}x + C = 0, \quad (62a)$$

where x is the B position of the carbon bond and ϕ is a configurational potential (Figure 2), and for coupling to 2d immediate neighbors:

$$E_W = |A|^2/4B \text{ is the depth of the local potential,} \quad (62b)$$

$$E_B = C|A|/Bd \text{ is the representative bond energy,} \quad (62c)$$

defining a constant $h = E_W/E_B$.

(62d)

For $h \gg 1$ only localized transitions occur, but for $h \ll 1$ a displacive transition (Bruce and Cowley, 1980; Murata, 1975; Aubrey, 1975, 1976;

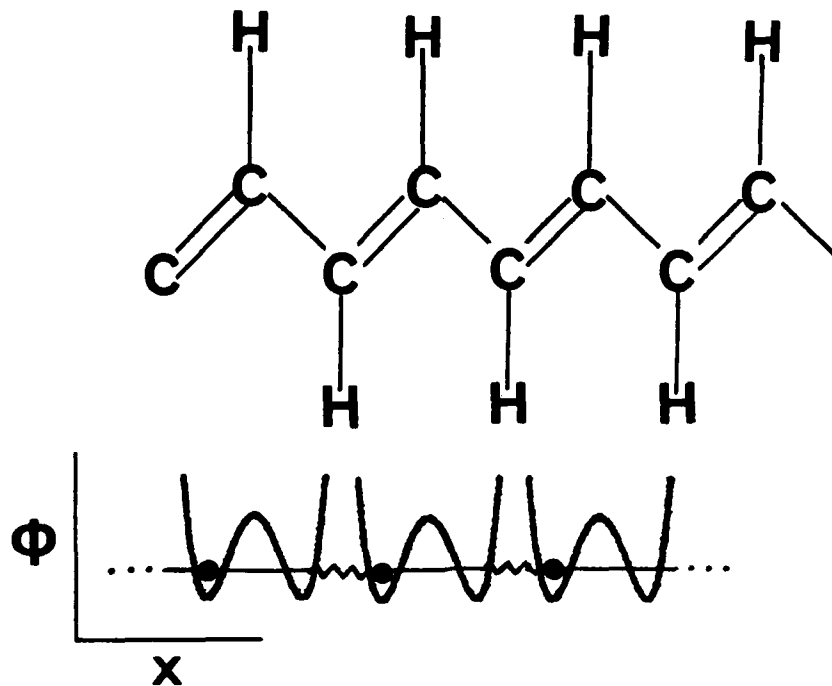


Fig. 17

McMillan, 1976; Hohenberg and Halperin, 1977; Halperin, Hohenberg and Ma, 1974; Halperin, Hohenberg and Ma, 1976) results in an incommensurate phase domain wall diffusion (soliton propagation).

To describe a propagating transition in a chain of monomers of the type depicted in Figure 17, the transition becomes displacive (Schneider and Stoll, 1973, 1975, 1976, 1978) ($h \ll 1$), resulting in domain wall diffusion.

The potential energy of the Hamiltonian description of the process is

(Bruce, 1978; Bruce and Cowley, 1980):

$$V = \frac{C}{2} \sum_{\ell, \ell'} \frac{n_{\ell} n_{\ell'}}{n_{\ell} n_{\ell'}} (u(\ell) - u(\ell'))^2 + \sum_{\ell} \phi(\ell), \quad (62e)$$

Taking into consideration that the doping process results in the previously mentioned competition with the hydrogen (state of resonance) for a carbon bond (Chen et al., 1978), then ideally the doping results in two

types of configuration, A and B (Figure 18). In the Figure 18A doping condition the bond transfer from left

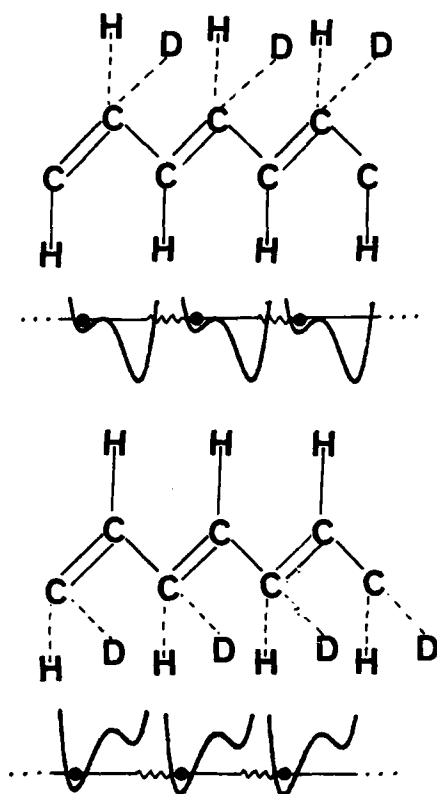


Fig 18

to right (effecting a transfer from one isomerized state to the other) is facilitated, as the dopant provides a stronger electron acceptance in the isomerized state to be adopted. In the Figure 18B doping condition, on the other hand, the bond transfer from left to right is less likely, as the dopant provides a stronger electron acceptance in the isomerized state already existing. The actual result of doping is more probably the nonideal forms shown in Figure 19, where the angle χ is a pictorial representation for the degree of resonance interaction of bond 1 with bond 2 and the depth of the configurational double potential well (Figure 20).

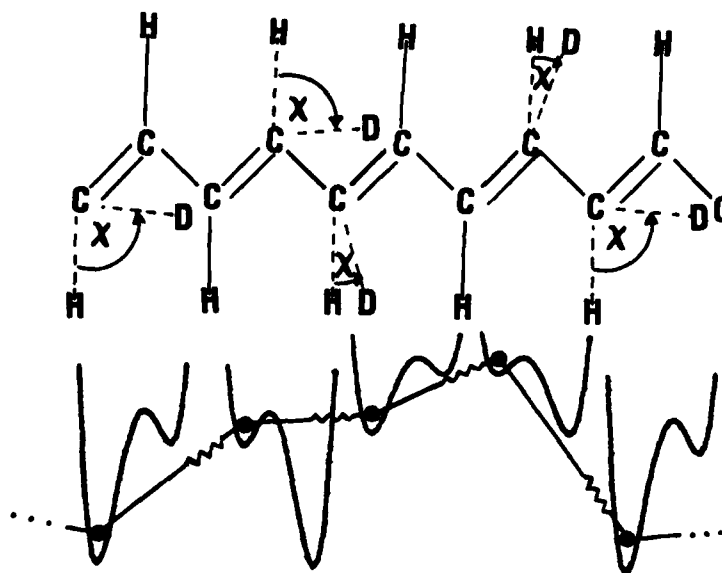


Figure 19

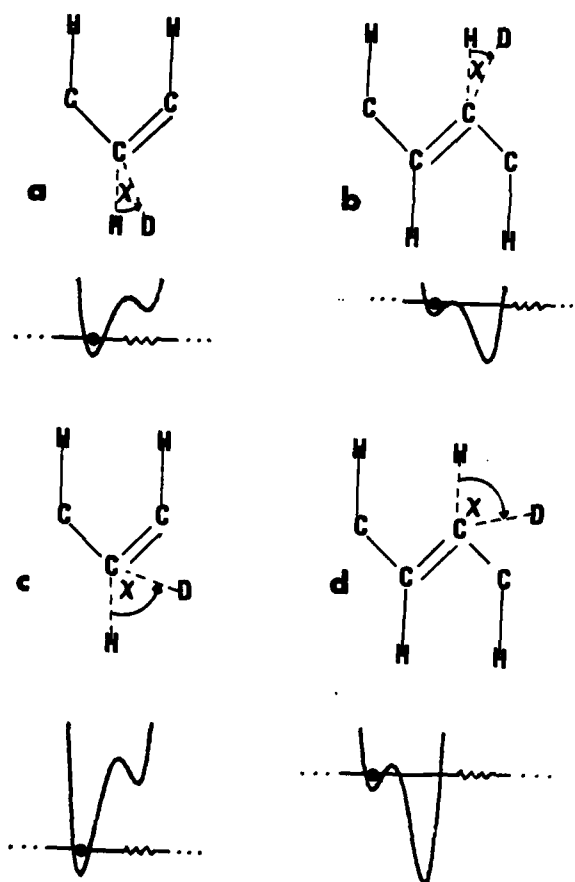


Figure 20

It is a consequence of the anharmonic oscillator model that any of the joined monomer segments shown in Figure 19 may be represented as a trajectory over the a, b surface representation of the monomer element dynamics described by Eq. (62a). In Figure 21 is shown an arbitrary semicircular trajectory; and Figure 22 depicts the possible nonuniform doping of $(CH)_x$ and monomer configurational potential wells for a complete circular trajectory. The particular trajectory is, of course, arbitrary, but for purposes of exposition the circular trajectory will be used here. In the case of trajectory $1 \rightarrow 8$, at each of the 8 monomer sites and for an increasing applied current to the $(CH)_x$ chain, the measured voltage, if it could be measured, would show an initial increase to V and then greatly diminishing increases after that value. Conversely, for an increasing applied voltage to the $(CH)_x$ chain, the measured current, if it could be measured, would show an initial slow increase until a ΔI value is reached and then increase greatly.

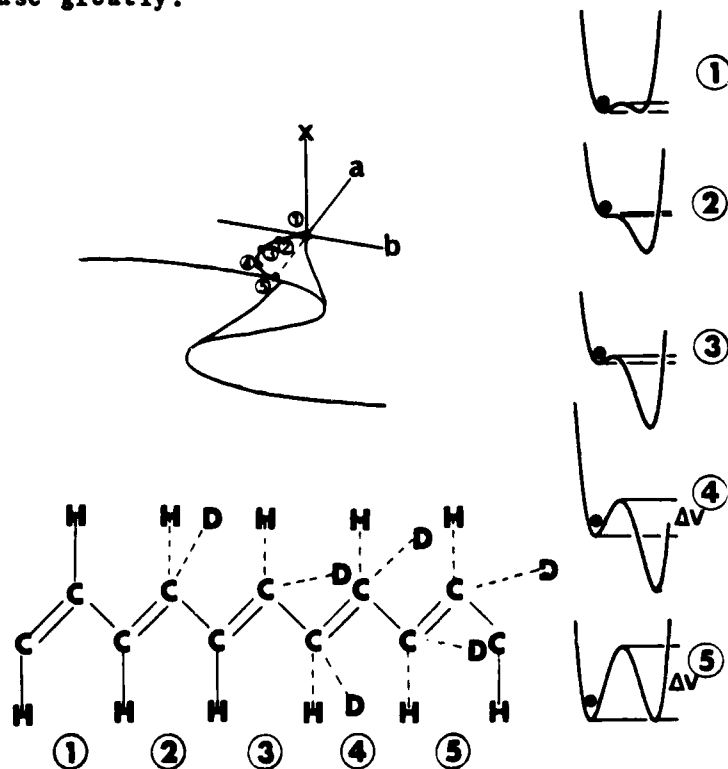


Fig. 21

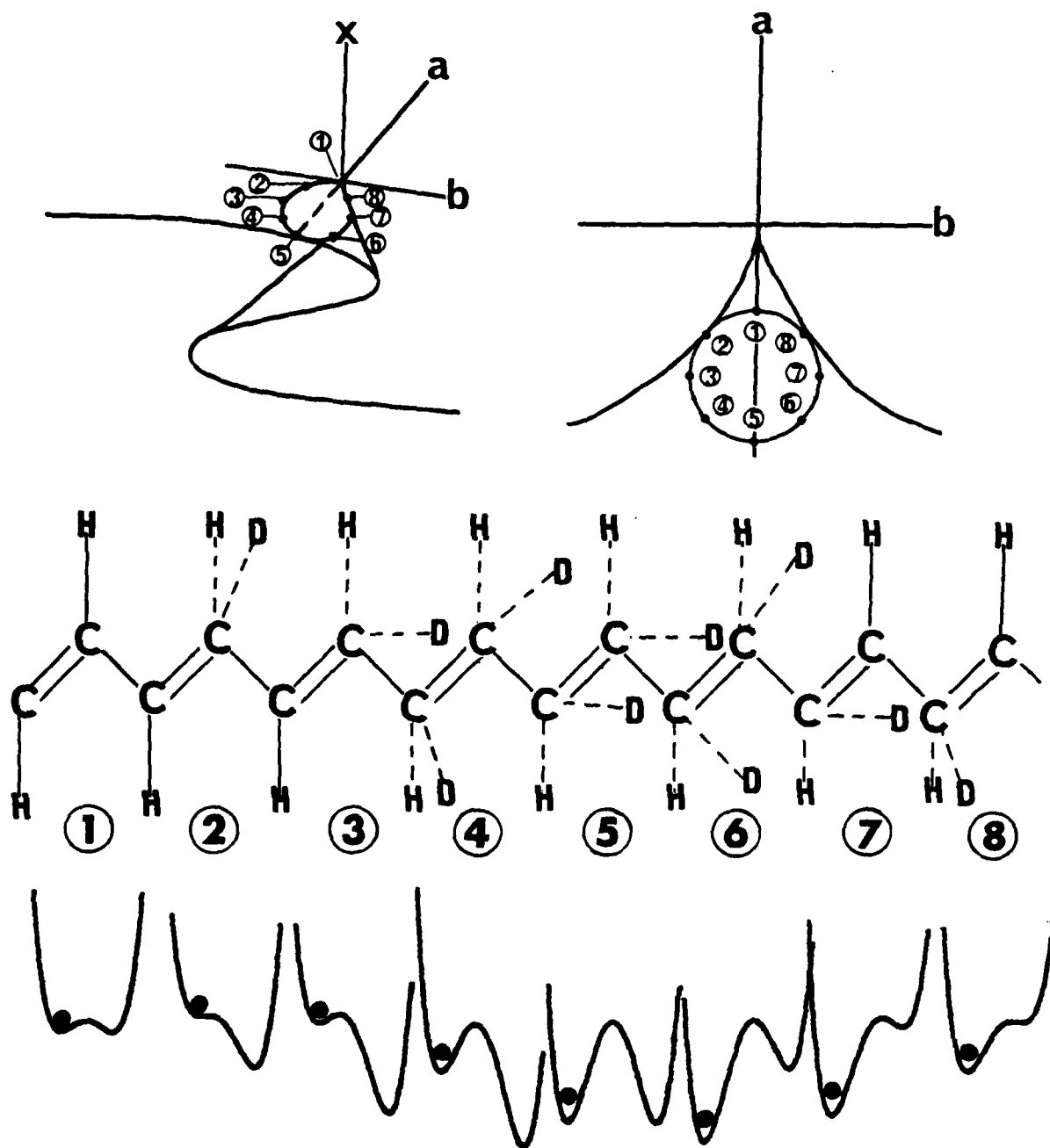


Figure 22

With constant current applied and the resistance and voltage measured at each monomer location, if such could be measured, the following relation would then be obtained (Figure 23):

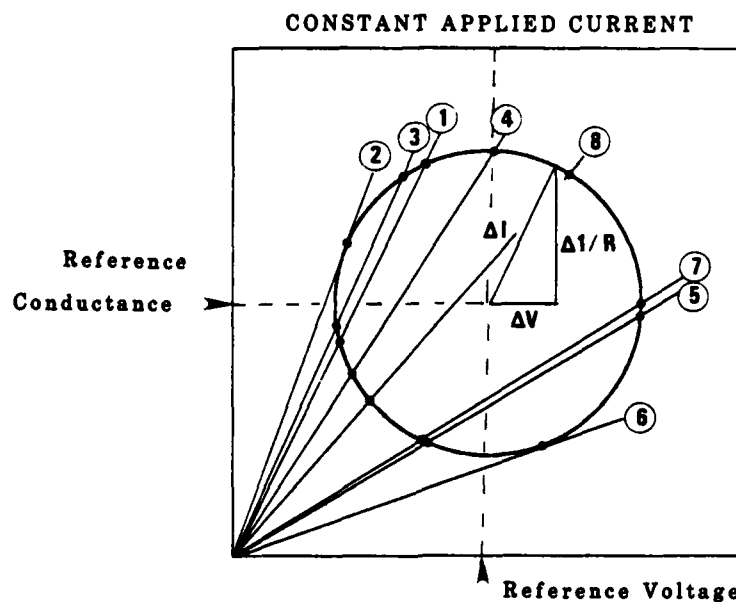


Fig. 23. Logarithmic representation of ΔV , $1/\Delta R$ and constant applied ΔI relations of the trajectory of Figure 22. The numbers refer to the locations in Figures 21 and 22.

For the particular nonuniformly doped chain considered, the monomer current-voltage relations at each monomer site would be (Figure 24):

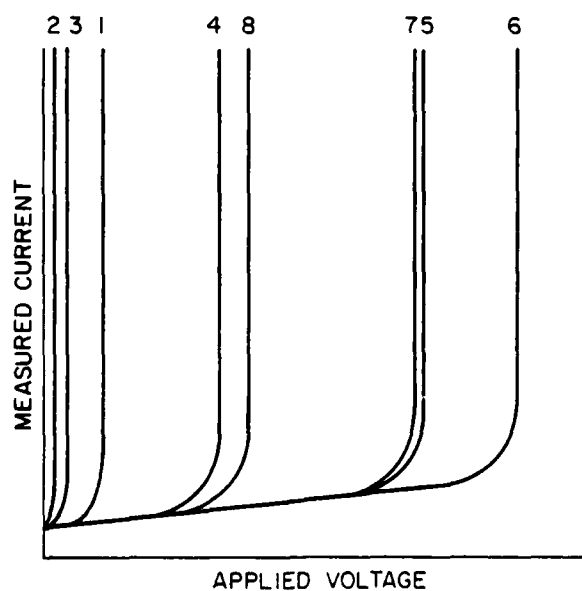


Fig. 24. Current singularities in the nonuniformly doped $(CH)_x$ chain for the locations in Figures 21 and 22.

There is little hope of measuring such monomer current-voltage relations presently. However, the task to relate the soliton-mediated conductivity at each monomer site to the conductivity which may be measured for a collection of such chains may be approached analytically. For example, $(\text{CH})_x$ chains consisting of monomers with less resistance, ΔR , should exhibit more solitons, at equal applied current, than chains with more such resistance.

It is demonstrated in the next section that relating the current-voltage quadratic relation problem to the d.c. current singularities of the long Josephson junction is straightforward, resulting in an explanation for the current-voltage relations of a collection of nonuniformly doped $(\text{CH})_x$ chains, as both phenomena are based on the same soliton dynamics.

c. Long Josephson Junction Analogy

The problem of predicting the average voltage for a given applied current in a nonuniformly doped $(\text{CH})_x$ chain is directly related to the explanation of the d.c. current singularities of the long Josephson junction (Chen et al., 1971; Parmentier, 1978; Parmentier and Costabile, 1978; Costabile et al., 1978; Costabile et al., 1980; Costabile and Parmentier, 1980) (Figure 25). The fluxon on the long Josephson junction is mathematically equivalent to a soliton and shares with the $(\text{CH})_x$ soliton a common analytical mechanics.

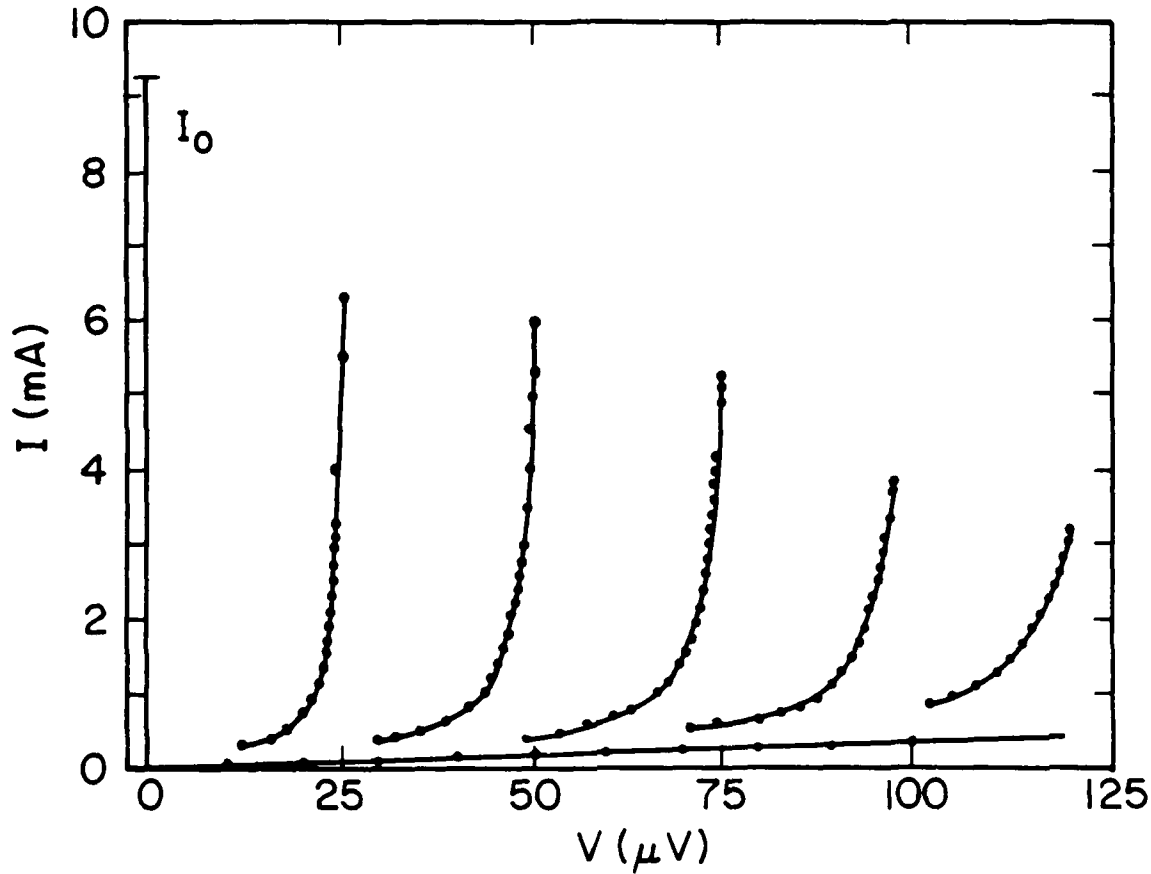


Fig. 25. Current-voltage characteristic of a very long Josephson junction showing zero-field current steps in the presence of an external magnetic field applied transversely across the junction. From Costabile et al., 1980.

The sine-Gordon equation, without dissipative effects for which the soliton is a solution, is:

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} = \sin \phi, \quad (62e)$$

where ϕ is the phase difference between macroscopic quantum wave functions that characterize two superconductors and is directly analogous to the ϕ of the anharmonic oscillator model. The soliton (fluxon) solution to Equ.

(62e) is (Lamb, 1971):

$$\phi = 4 \tan^{-1}(f(x)g(t)), \quad (62f)$$

and f and g are Jacobian elliptic functions defined (Chen et al., 1971; Parmentier, 1978; Parmentier and Costabile, 1978; Costabile et al., 1978):

$$\frac{df}{dx}^2 = Af^4 + (1+B)f^2 - C, \quad (62g) \text{ (i)}$$

$$\frac{dg}{dt}^2 = Cg^4 + Bg^2 - A, \quad (62g) \text{ (ii)}$$

where A , B and C are arbitrary constants. Taking $a = (1+B)/A$, $b = C/A$ for Equ. (i) and $a = B/C$, $b = A/C$ for (ii), and differentiating, the form of Equ. (62a) is obtained.

For the case of most interest, that with dissipative effects, we have:

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} - \alpha [1 + \cos \phi] \frac{\partial \phi}{\partial t} = \sin \phi, \quad (62h)$$

where α and ε are constants. This form can be solved by assuming an x and t dependence of ϕ , e.g.:

$$\phi = \phi(x - ut) = \phi(\xi), \quad (62i)$$

where u is a constant propagation velocity.

With α and ε related to an external energy source, Equ. (62g) is:

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} - \Gamma (1 + \cos \phi) \frac{\partial \phi}{\partial t} \bigg| \frac{\partial \phi}{\partial t} = \sin \phi - \gamma, \quad (62j)$$

where $\Gamma = g_0 \phi_0 / 2\pi C$,

$$\varepsilon = g_1 / g_0,$$

$$\gamma = I_B / I_0,$$

$$\alpha = g_0 |v| (\phi_0 / 2\pi I_0 C)^{1/2}$$

and I_B is a uniformly distributed current bias for the long Josephson junction and a current bias for the $(CH)_x$ chain.

With this external source dependence, Equ. (62j) has the desired quadratic current-voltage characteristic with normalized voltage (Parmentier, 1978):

$$v = \frac{1}{\pi k} \left(\frac{\gamma_0}{2\Gamma} \right)^{1/2} \operatorname{dn} \left[\frac{1}{k} \left(\frac{\gamma_0}{2\Gamma u^2} \right)^{1/2} (\xi - \xi_0); k \right], \quad (62k)$$

where ξ_0 is an arbitrary constant;

$$\xi = (x - ut);$$

and $\operatorname{dn} [;]$ represents a Jacobian elliptic function (Lamb, 1971) of modulus

$k, 0 < k < 1;$

$$k = \left(\frac{2\gamma_0}{\gamma + \gamma_0} \right)^{1/2}; \quad (62i)$$

$$\gamma_0 = 2\Gamma u^2 [(1-u^2)^2 + 4\Gamma^2 u^4]^{1/2}. \quad (62m)$$

Because

$$\frac{1}{k} \left(\frac{\gamma_0}{2\Gamma u^2} \right)^{1/2} = 2nK(k), \quad (62n)$$

where ℓ is the length of the long Josephson junction (or $(CH)_x$ chain;

$K(k)$ is the complete elliptic integral of the first kind; and n is the number of solitons (fluxons contained on it), the average value of voltage, v , is:

$$\langle v \rangle = nu/\ell. \quad (62o)$$

As the number of solitons, n , will vary from monomer to monomer at constant applied current, depending on the doping conditions, the average $\langle n \rangle$ is substituted for n and:

$$\langle v \rangle = \langle n \rangle u/\ell. \quad (62p)$$

The current-voltage relations calculated with Equ. (62p) are shown in Figure 26. The similarity between the relations shown in Figure 26, the

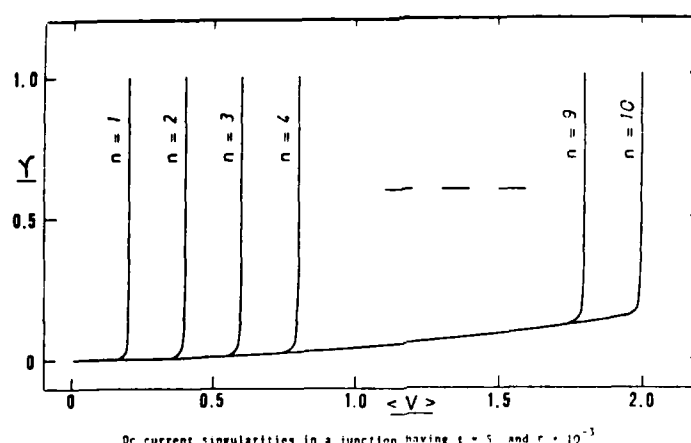


Fig. 26. Current-voltage characteristics for n fluxon oscillations. From Parmentier, 1978. Fluxon oscillations move to one end of a long Josephson junction are reflected as an antfluxon and move to the other end, etc. (Fulton and Dynes, 1973). Such oscillations can adsorb power from an external source of bias current. Costabile et al. (1978) have also made similar calculations using an approximation scheme rather than an exact solution with periodic boundary conditions.

putative relations of Figure 24 and the experimentally obtained relations of Figure 16, indicate that a possible explanation of the nonlinearity of Figure 16 is obtained.

X. THE IMPORTANCE OF SYMMETRY BREAKING

In previous sections, the precise underlying dynamics of each link in the polyacetylene chain was addressed. The behavior of such a one-dimensional conductor in T-junction form was described (section I-III) and the effect of uneven doping and the application of Ohm's and Kirchoff's laws to these systems predicted (sections IV-IX).

In this section, two facets of the one-dimensional organic conductor problem are addressed. The first is a description of how the conditions for the underlying dynamics of soliton propagation may arise, and we show that these conditions are caused by broken symmetry, placing the problem squarely in the frame of modern critical phenomena theory.

The description of this first facet leads to a description of the second, which is the relation of our present description of every link in the polyacetylene chain to the more manageable Hubbard model (Hubbard, 1963, 1964a,b) and its developed form (Economou, White and DeMarco, 1978; White and Economou, 1978; DeMarco, Economou and White, 1978). In achieving a description of the second facet of the underlying dynamics, the problem is placed in the frame of current correlation techniques for describing conduction and magnetism based on the double-time Green function method of Zubarov (1960) (section XI below). In effect, this reduces the nonlinear many-body problem addressed in sections I-IX to a one-body one.

In reducing the many-body problem to one-body (Hubbard) form, we see advantages and disadvantages. One advantage is the obtainment of a more manageable Hamiltonian and in relating this development to mainstream

theories of conduction. A disadvantage, however, is that the underlying dynamics is introduced somewhat artificially to the essentially static one-body description with a resulting decrease in physical insight. Thus, we recommend that only the sections I-IX and present, taken together, achieve an in depth description of the underlying dynamics.

The following is a general description of symmetry breaking at both the micro and macrophysical levels beginning with a description of polymer monomer described by the Schrödinger-like equation (20) of section IV:

$$\ddot{\phi} = f_0^2 + af_0 + b = 0, \quad (62b)$$

where f_0 may be taken as the midfrequency of a signal equivalent to electron momentum in the analysis of states. The procedure is to demonstrate that a system described by an equation similar to that of Eq. (62) not only exhibits two potential minima (isomerization) when the variable, a , is negative (which is known), but that, more importantly, a negative variable, a , results in symmetry breaking.

In order to achieve this aim, some conclusions are first summarized before (Barrett, 1977, 1978, 1979a,b.,1980) pertaining to any system described by an equation similar to Eq. (62).

a. Although never stated as a logical consequence of any deeper theoretical condition, the fundamental conditions for the valid application of quantum mechanics are the commutation relations (Dirac, 1967; Heitler, 1954; Schiff, 1973; Louisell, 1973):

$$\begin{aligned} q_r q_s - q_s q_r &= 0, \\ p_r p_s - p_s p_r &= 0, \\ q_r p_s - p_s q_r &= i\hbar \delta_{rs}, \end{aligned} \quad (63)$$

where the operators q and p are canonical coordinates and momenta and r and s refer to degrees of freedom, $r = s$. With one degree of freedom, the commutation relation is:

$$qp - pq = i\hbar. \quad (64)$$

b. The supposition of this commutation relation enables, using the Schwartz inequality, the following uncertainty condition to be described involving the numbers, Δp and Δq , defined as standard deviations about p and q :

$$\Delta p \Delta q = 1/2\hbar. \quad (65)$$

Because, just as readily, the following commutation relation might be supposed involving the operators, Δp and Δq :

$$\Delta q \Delta p - \Delta p \Delta q = i\hbar, \quad (66)$$

then we arrive by similar reasoning at the uncertainty relation for the numbers, p and q (Barrett, 1977):

$$p \cdot q = 1/2\hbar, \quad (67)$$

thereby defining the quantum condition as a four-parameter condition in which the concept of number or operator is considered relative.

c. Because of logic used to solve the Schrödinger equation and to define the energy eigenfunctions of states of the harmonic oscillator could as easily, and in the long run more appropriately, define signals produced by a harmonic oscillator (i.e., the uncertainty relations might be derived as a condition for the solution of a harmonic oscillator - this is admitted as possible in some texts, e.g., (Schiff, 1973, p. 73), we have then the possibility of more general relations.

Because: (i) In the root-mean-square deviation from the mean, or expectation value, $(\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2$,

$$(\Delta q)^2 = \langle (q - \langle q \rangle)^2 \rangle = \langle q^2 \rangle - \langle q \rangle^2,$$

and (ii) as $\langle p \rangle = \langle q \rangle = 0$ for any harmonic oscillator wave function, then (i) permits us to write:

$$(\Delta p)^2 = \langle p^2 \rangle,$$

$$(\Delta q)^2 = \langle q^2 \rangle.$$

(iii) If fluctuations are now introduced, not to p and q in the sense of defining Δp and Δq , but to Δp and Δq in the sense of defining p and q , then, in analogy to (i):

$$\langle p \rangle^2 = \langle \Delta p - \langle \Delta p \rangle \rangle^2 = \langle \Delta p^2 \rangle - \langle \Delta p \rangle^2,$$

$$\langle q \rangle^2 = \langle \Delta q - \langle \Delta q \rangle \rangle^2 = \langle \Delta q^2 \rangle - \langle \Delta q \rangle^2,$$

i.e., if p and q are thought of as types of carrier signals and Δp and Δq as types of modulating envelopes of those signals, then (i) above describes fluctuations in the carrier signals and here in (iii), fluctuations in the modulating envelopes are described.

(iv) Thus, in analogy to (ii): $\langle \Delta p \rangle = \langle \Delta q \rangle = 0$ for any modulated harmonic oscillator, and (iii) permits us to write:

$$\langle p \rangle^2 = \langle \Delta p \rangle^2,$$

$$\langle q \rangle^2 = \langle \Delta q \rangle^2.$$

We then have the two uncertainty products for the modulated harmonic oscillator:

$$\Delta p \cdot \Delta q = 1/2(2n + 1)\hbar: p \cdot q = 1/2(2n + 1)\hbar, n = 0, 1, 2, \dots \quad (68)$$

The physical significance of this viewpoint is that an uncertainty relation may arise either from inherent fluctuations in the oscillator or in fluctuations in the external modulation of the oscillator.

d. With an emphasis on the signal-like character of the uncertainty products, which in acoustics can be used as signals, it is easier to treat f_0 , or signal midfrequency, instead of p , Δf , or signal bandwidth, instead of Δp , t_0 , or signal midperiod, instead of q , and Δt , or signal duration, instead of Δq .

This permits the following relation for quantal signals in a way identical to the uncertainty product derivation of c:

$$f_0 \cdot t_0 = 1/2c(2n + 1), n = 0, 1, 2, \dots, \quad (69a)$$

$$\Delta f \cdot \Delta t = 1/2c(2n + 1), n = 0, 1, 2, \dots, \quad (69b)$$

$$\Delta f = f_0/f, \Delta t = 4t_0, \text{ for } n = 0, \quad (69c)$$

$$\Delta f \cdot \Delta t / f_0 \cdot t_0 = 1, \quad (69d)$$

i.e., a constant magnetic field influence is assumed (constant modulation), n is the angular momentum quantum number, $c = \hbar$ for wave optics or reception by a radially circulating receiver, and $c = 1$ for wave acoustics or a linearly acting receiver.

e. The wave packet or quantal signal for light and sound with $n = 0$ is:

$$s(t) = \exp[-(1/c)(t - t_0)^2] \exp[i2\pi f_0 t] \text{ in the time domain,} \quad (70a)$$

$$S(f) = \exp[-c(\pi)^2(f - f_0)^2] \exp[-i2\pi t_0 f] \text{ in the frequency domain.} \quad (70b)$$

In general, the signals are:

$$s(t) = D_n(t) \cos(180t^{1/2}(2n + 1))^\circ, n = 0, 1, 2, \dots, \quad (71)$$

where the $D_n(t)$ are modified Weber-Hermite polynomials:

$$D_n(t) = \exp[(-1/2c)t^2] H_n(t), n = 0, 1, 2, \dots \quad (72)$$

and the $H_n(t)$ are Hermite polynomials:

$$H_n(t) = (-1)^n \exp[t^2] \partial^n \exp[-t^2] / \partial t^n, n = 0, 1, 2, \dots \quad (73)$$

The equations expressed in Eqs. (69) are the solutions to the wave amplitude equation for the harmonic oscillator system (i.e., to Schrödinger's equation). A formally similar equation to the Schrödinger equation relates all four, but only those four, signal parameters has been shown to be (Barrett, 1977):

$$f_0^3 - (-4\Delta f^2 \Delta t / t_0) f_0 + (-16\Delta f^2 / t_0) = 0, \quad (74)$$

This, in turn, is example of the well-studied equation for a harmonic oscillator:

$$\ddot{\phi} = f_0^3 + af_0 + b = 0, \quad (75)$$

or the differential of:

$$\phi = 1/4f_0^4 + 1/2af_0^2 + bf, \quad (76)$$

where ϕ is a potential function.

f. In Figs. 28 and 29 curves of ϕ vs. f_0 are plotted, demonstrating that, within a certain range of $a = 4\Delta f^2\Delta t/t_0$ and $b = -16\Delta f^2/t_0$ values, two potential minima are available, and the quantum effect is inseparable from the existence of an area of instability defined by the presence of more than one potential minimum.

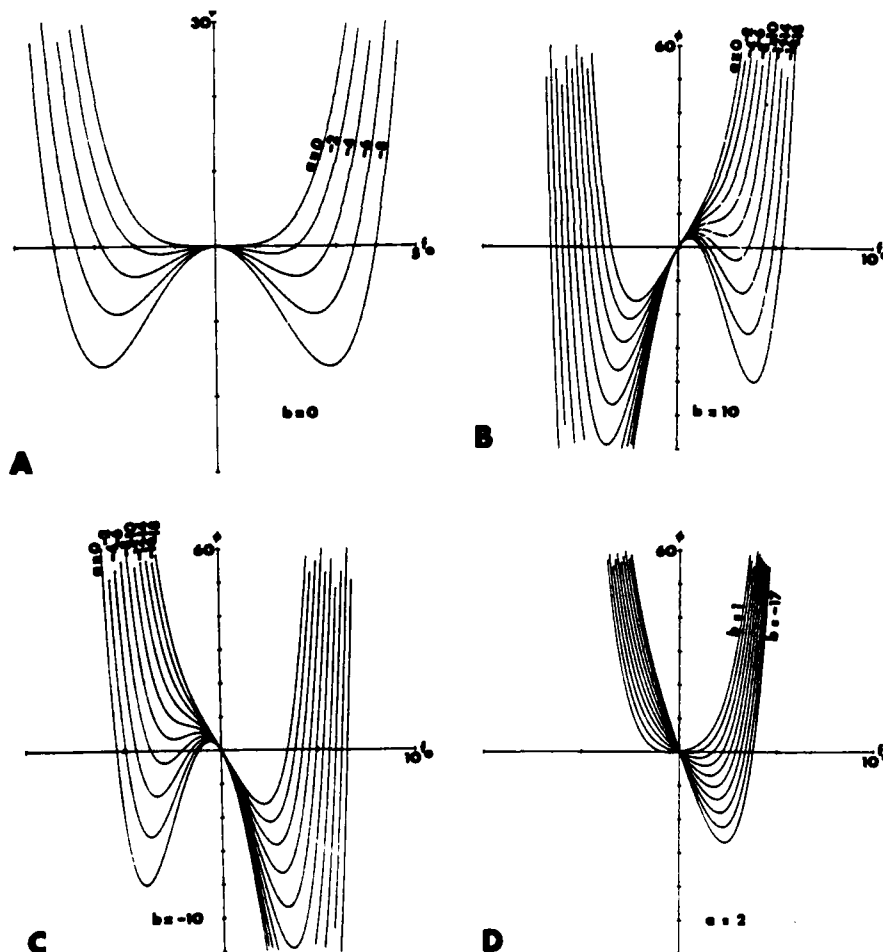


Figure 28

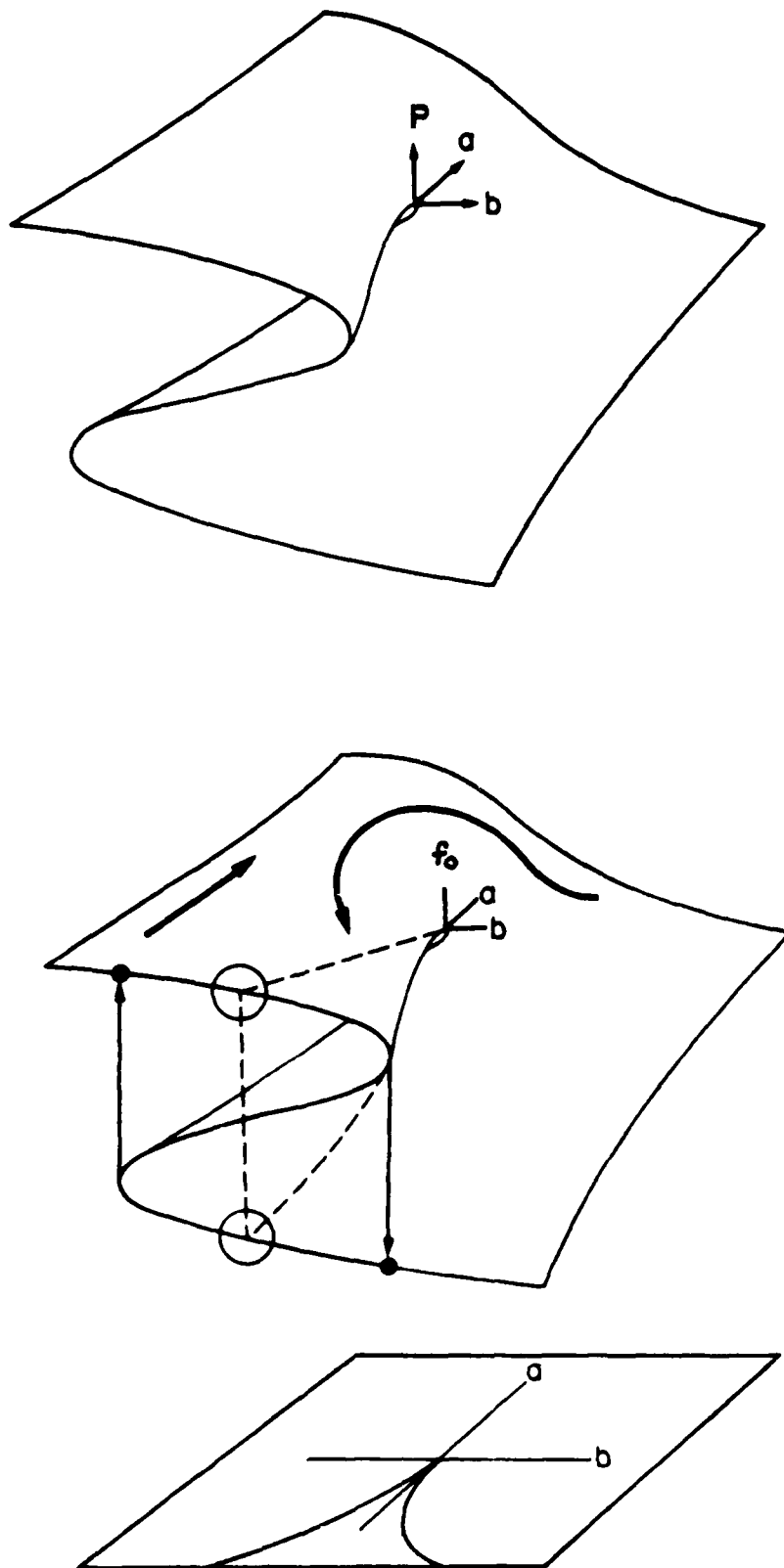


Figure 29

Here, the intention is to demonstrate that these two potential minima define the location of two fixed points: the Gaussian and a nontrivial fixed point, where a fixed point is defined in the terms of renormalization group theory (Pfeuty and Toulouse, 1977; Wilson, 1971) as a point in parameter space which by itself constitutes its own entire trajectory. To such a point there corresponds a state of the system invariant under the operations of the renormalization group and which has a correlation length either infinite or zero (Pfeuty and Toulouse, p. 13).

(i). Argument

In the vicinity of a transition point between a stable region (defined by one fixed point, the Gaussian) and an unstable region (defined, as above, by two fixed points, one of which is the Gaussian), there are fluctuations which govern the behavior of the system. Close to the critical point quantities may be observed which obey power laws with exponents that are not integers. For example, just below T_c , the critical temperature, the order parameter (f_0) begins by falling proportionately to $(T_c - T)^\beta$, while just above T_c the specific heat, for instance, is proportional to $(T - T_c)^{-\alpha}$, the correlation length to $(T - T_c)^{-\nu}$, and the susceptibility, in the case of a magnetic system, to $(T - T_c)^{-\gamma}$. The exponents α , β , ν , γ , and others are defined in the vicinity of a given critical point, and are called critical exponents. These critical exponents obey some simple relations called scaling laws, which have a degree of universality. In the case of a magnetic system, the scaling laws are satisfied automatically if the singular part of the free energy $G(T - T_c, H)$ and the correlation function $\Gamma(T - T_c, \underline{R})$ are homogeneous functions of their arguments.

In the case of a magnetic system, for the equation of state there exists a law of corresponding states interrelating the order parameter.

M, its conjugate field, H, and the temperature, $(T - T_c = \tau)$ by an equation of the form (Stanley, 1980):

$$H/M^\delta = h(\tau/M^{1/\beta}) \quad (77)$$

In the case of the quantal system defined by Eqs. (69), this is:

$$t_0/f_0^\delta = h(\Delta t/f_0^{1/\beta}). \quad (78)$$

With $\delta = 1$ and substituting $c = 1$ for h , the relations expressed by Eqs. (69) and (78) give a value for β of $\log(f_0)/\log(4f_0)$, e.g. 0.6 for $f_0 = 8$. In the case of the relations expressed by Eqs. (1), $\beta = \log(p)/\log(4hp)$.

In terms of a modulated harmonic oscillator, Equ. (78) describes the relation of the midperiod of oscillation (f_0), the midperiod of oscillation (t_0), and the temporal window of modulation (t), for the case of the minimum quantum ($n = 0$, Equ. (69) at different β s ($= \log(f_0)/\log(4f_0)$) or different f_0 s. A similar description holds for p and Δp for the case of the minimum quantum ($n = 0$, Equ. (68)) and different p 's.

From Widom's scaling law (Pfentz and Toulouse, 1977, p. 22):

$$\gamma = \beta(\delta - 1), \quad (79)$$

we have, for the present system, $\gamma = 0$. From Rushbrooke's scaling law:

$$\alpha + 2\beta + \gamma = 2, \quad (80)$$

we obtain $\alpha = 0.8$ for $f_0 = 8$, or $\alpha = 2 - 2\log(f_0)/\log(4f_0)$ generally, and from Fisher's scaling law:

$$\gamma = (2 - n)\nu, \quad (81)$$

either $\nu = 0$ or $n = 2$. As Josephson's scaling law:

$$\nu d = 2 - \alpha \quad (82)$$

must be satisfied, $n = 2$. With $d = 4$, which corresponds to $a = 0$ (of Equ. (62): $f_0^3 + af_0 + b = 0$), Equ. (82) gives $v = 0.3$ for $f_0 = 8$, or $v = 1/2 \log(f_0)/\log(4f_0)$ generally. Within the area of instability, then, $a < 0$, $d < 4$ and $v > 1/2 \log(f_0)/\log(4f_0)$, for the quantal system considered with the correlation length, ξ , defined:

$$\xi \sim \frac{1}{|\Delta t|v} \quad (83)$$

Josephson's law, $vd = 2 - a$, links the space dimensionality, d , the exponent, a , referring to a thermodynamic potential and the exponent v referring to a correlation function. As d decreases through the value $d = 4$, one moves from a regime ($d > 4$, $a > 0$), where Josephson's law fails, to another regime ($d < 4$, $a < 0$), where it holds. The mathematical basis for this lies in the simple identity, $-a = 4 - d$ (where a is defined in Equ. (62)), or, as is generally given, in the expansion parameter $\epsilon = 4 - d$ (Hohenberg and Halperin, 1977), i.e., $\epsilon = -a$.

The relation of the space dimensionality d to the parameter a of Equ. (74) is seen clearly in Fig. 30 and in recent developments in renormalization group methods (as reviewed in (Hohenberg and Halperin, 1977)). These methods include 1) reduction of the number of degrees of freedom, 2) restoration of the spatial density of degrees of freedom to its initial value, and 3) renormalization of spin magnitude, if appropriate to do so. Referring to Fig. 31, a comparison of two systems, 1 and 2, can be obtained if a , is renormalized to equal a_2 (for the systems $f_0 + a_i f_0 + b_i$, $i = 1, 2$). The two systems would then be located at the same position along the a axis and comparisons of the two systems could be made along the f_0 and b axes. This is, then, the essence of the renormalization approach.

If elementary particle behavior is considered, then the particle only exists in the region $d < 4$, $a < 0$, due to the energy minimization

requirement for the solution of a harmonic oscillator given in $X(c)$. To ask, therefore, whether an elementary particle could exist in the classical domain ($d > 4$, $a > 0$) is to ask whether the energy minimization requirements could be disregarded.

A formal analogy can be developed for another example using the solution to the percolation problem by Fortuin and Kasteleyn (1972). This application illustrates the generality of the mathematical system generated by broken symmetry, i.e. the dynamic underlying both the quantum harmonic oscillator and the percolation problem is formally similar. The percolation problem considers an infinite lattice whose sites are, at random, either allowed or forbidden, with a probability, p , that any given site is allowed. A critical value, p_c , is defined so that when $p \geq p_c$, there occurs an infinitely large cluster of allowed sites and percolation takes place, i.e., one can cross the lattice by going successively from one allowed site to a neighboring allowed site. In the present instance, and also in the case of ferromagnetism, we let $(p - p_c) = (t - t_0) = \Delta t$. Other formal mathematical correspondences are:

a. The probability, M , that an allowed site belongs to an infinite cluster is equivalent to the frequency, f_0 , in the present case, and to spontaneous magnetization in the ferromagnetic case,

b. The average size of finite clusters is equivalent to the susceptibility in the ferromagnetic case and will be shown to be unity in the present case, and

c. The average number, G , of clusters is equivalent to the free energy in the ferromagnetic case and will be shown to have a value in the present case when $n \neq 0$.

For the general case expressed by Eqs. (7) and (9), the average number of signals of size n is:

$$G(t, n) = \frac{t \cdot G(t, n)}{t}, \quad (84)$$

and the average number of signals having any size is:

$$G(t) = \sum_n G(t, n). \quad (85)$$

Then, the average size of finite signals (susceptibility) is:

$$\chi(t) = \sum_n n^2 G(t, n), \quad (86)$$

or:

$$\chi(t) \sim \left(\frac{1}{\Delta t}\right)^\gamma, \quad (87)$$

whence we see that for G and χ to be other than unity, $\gamma = 0$ or $\delta \neq 0$ or $n \neq 0$.

The percolation problem solution also gives:

$$f_0 \sim \Delta t^\beta, \quad (88)$$

which is satisfied by Equ. (69) for $\beta = \log(f_0)/\log(2/f_0)$.

We turn now to the role of broken symmetry in the transition from classical to quantum mechanics. The Ginzburg criterion describes the existence of a characteristic dimensionality below which fluctuations are so large that, in the vicinity of the critical point, the self-consistency of the classical theory of mechanics is destroyed, resulting in a broken symmetry for certain rotations and the necessity of a quantum mechanical formulation. This amounts to defining B , the coefficient of the quartic term in the usual expression for free energy ($F = A \cdot M^2 + B \cdot M^4 + k(\nabla M)^2$), as:

$$B \sim (\Delta t)^{(4-d)/2}. \quad (89)$$

On the other hand, we have previously defined the area of instability (in which two potential minima exist, not one minimum) as extending from $b = +1.3$ (cf. Fig. 28), where b is defined in Eqs. (75) and (76) ($f_0^3 + a f_0 + b = 0$). In the normalized units of Fig. 28, Δt is 0.147,

and for $d = 4, 5, 6, 7, 8, \dots$, we have $B = 1, 3, 7, 18.5, 46.3, \dots$

To describe the Hamiltonian of a system capable of broken symmetry, we let $\Delta t \simeq r_0$ (more generally, $r_0 \sim \Delta t((1 + \Delta t + \dots) + (\Delta t)^{2/(d-2)}(1 + \Delta t + \dots))$) and $B \simeq u_0$. The system Hamiltonian is then:

$$H = \mu_0 + 1/2 \int_{k < 1/2} (r_0 - k^2) f(k)^2 + \quad (90)$$

$$\mu_0 \int_{k_1, k_2, k_3, k_4 < 1/2} f(k_1) \cdot f(k_2) \cdot f(k_3) \delta(k_1 + k_2 + k_3 + k_4).$$

where a is a unit of length for the system, or lattice spacing. Any dilatation of this unit of length requires renormalization of the Hamiltonian, and the parameters r_0 and u_0 renormalize (Wilson, 1971) subject to the differential equations:

$$\frac{dr_0}{d\ell} = 2r_0 + bu_0(1 - r_0), \quad (91a)$$

$$\frac{du_0}{d\ell} = \varepsilon u_0 - cu_0^2, \quad (91b)$$

where $\varepsilon = 4 - d$, $b = 16(n + 2)$, and $c = 16(n + 8)$, and $s = e^\ell$, for the dilatation $a \rightarrow sa$. Eqs. (91), set to zero, yield two solutions. The first, $(r_0^* = u_0^* = 0)$, corresponds to the Gaussian fixed point, and the second, $(r_0^* = -\frac{b}{2c} \varepsilon; u_0^* = \frac{\varepsilon}{c})$, corresponds to the nontrivial fixed point. In the neighborhood of each fixed point $r_0 = r_0^* + \delta r_0$ and $u_0 = u_0^* + \delta u_0$ permitting the definition of a matrix A_g for the Gaussian fixed point:

$$A_g = \begin{pmatrix} 2, & b \\ 0, & \varepsilon \end{pmatrix}$$

with eigenvalues $y_1 = 2$ and $y_2 = \varepsilon$, and a matrix A_{nt} for the nontrivial fixed points:

$$A_{nt} = \begin{bmatrix} (2 - \frac{b}{c\varepsilon}), & b(1 + \frac{b}{2c\varepsilon}) \\ 0, & -\varepsilon \end{bmatrix},$$

with eigenvalues $y_1 = 2 - \frac{be}{c}$ and $y_2 = -\epsilon$. For the simplest system described by Equ. (69), $n = 0$ and $y_1 = 2 - \epsilon/4$ and $y_2 = -\epsilon$, in the case of the nontrivial fixed point.

This development permits an important analogy between wave mechanics and lattice behavior i.e., the underlying dynamics of these two distinct physical phenomena have a similar mathematical form. The quantum system we are considering is based on an expansion in terms of n , the angular momentum quantum number (cf. Eqs. (69), (70), (71), and (72)). Another way of considering this description is to identify n with a lattice symmetry index or degree of isotropy (Fisher, 1974). In this alternative description, we commence with a lattice with sites \underline{x} populated with spins, $S_{\underline{x}}$, and we suppose the spin vector has n components, i.e., $S_{\underline{x}} = (S_{\underline{x}}^{\mu})$, $\mu = 0, 1, 2, \dots, n$, which enter equally into interactions. The case $n = 0$ describes the statistics of a self-avoiding walk or polymer chain in solution (de Gennes, 1972), $n = 1$ described the uniaxial or Ising model, $n = 2$, the XY or planar model, and $n = 3$, the Heisenberg model. The general model is the eight-vertex model of Baxter (Baxter, 1971). In this case, there are eight possible different configurations of arrows (spins) at each vertex. If a given eight-vertex model has a phase transition, then the free energy per vertex has a branch-point singularity.

The eight-vertex model has been shown to be equivalent to two Ising models with nearest neighbor coupling interacting with another via a four-spin coupling term (Kadanoff and Wegner, 1971; Wilson and Fisher, 1972). For $n > 4$, a "biconical" fixed point describing a tetracritical fixed point appears (Nelson, Kosterlitz and Fisher, 1974). An extension to the Weiss model (Weiss, 1907) for ferromagnets is also possible (Reidel and Wegner, 1969). In this instance, the entropy S per spin depends on the

square of the magnetization:

$$m^2 = m_{||}^2 + m_{\perp}^2, \quad (92)$$

to obtain:

$$S = S_0 - \frac{2}{2} m^2 - \frac{b}{4} m^4 + \dots \quad (93)$$

The free energy per spin:

$$F = E - TS, \quad (94)$$

where

$$E = 1/2 I_0 (m_{||}^2 + (1 - \Delta) m_{\perp}^2), \quad (95)$$

is differentiated to obtain the equations of state:

$$\frac{\partial F}{\partial m_{||}} = m_{||} (aT - I_0 + bT m^2) = h_{||}, \quad (96)$$

$$\frac{\partial F}{\partial m_{\perp}} = m_{\perp} (aT - I_0(1 - \Delta) + bT m^2) = h_{\perp}. \quad (97)$$

For $h_{||} = 0$, the paramagnetic region is defined by:

$$m_{||} = 0, \quad (98)$$

and the ferromagnetic region by:

$$aT - I_0 + bT m^2 = 0. \quad (99)$$

On the λ -line (Reidel and Wegner, 1969) both conditions described by Eqs.

(98) and (99) hold, and

$$\tau_{\lambda} = - \left(\frac{h_{\perp}}{I_0} - \frac{1}{\sigma} \right)^2, \quad (100)$$

where τ is the reduced temperature and $\sigma^2 = a/b$.

This development may be extended to include a description of ferromagnets with a Hamiltonian of cubic symmetry (Aharony, 1973), due to the presence in the Hamiltonian of single ion terms which reflect the lattice symmetry, thus breaking the full rotational invariance. For $d = 3$, $n \geq 3$, a crossover from isotropic (Heisenberg) to characteristic cubic behavior occurs, and there is an approximation to the behavior of the Fe^{2+} ion in the hemoglobin molecule. The benefit to be obtained from this analogy between wave mechanical systems and lattice systems is that the

physics of the latter predicts phase changes in the former under appropriate conditions.

The general model may also include the assumption that for only $d - m$ coordinates is there a contribution to the free energy density, which is quadratic in the spatial derivatives of the order parameter, f_0 (Hornreich, Luban and Shtrikman, 1975). In this case, the classical-quantum mechanical boundary is given by $d = 4 + m/2$. However, for clarity's and simplicity's sake, we shall assume that $m = 0$ here.

ii. Summary of (i)

The circumstances giving rise to the conditions described by Equ. (1) are general and are those of critical phenomena.

The potential, ϕ (Eqs. (20), (63) and (76)), the minimization of which results in an equation formally equivalent to the Schrödinger equation, can, in another formal analogy, be identified with the exchange energy at the vertex of a lattice. This indicates that the one-dimensional problem represented by polyacetylene can be generalized to n -dimensions.

The transition point defining the boundary between single and two state behavior is then quite definite: the boundary is at $d = 4$. For $d \geq 4$, we have single states, and for $d < 4$, we have two states due to the breakage of symmetry.

The principal quantum number and angular momentum quantum number (n) of elementary particle systems are equivalent to the dimensionality of space (d) and the dimensionality of the spin space (n) for n -vector spins of the general theory of critical phenomena. Turning this analogy around: we may use the general theory to indicate the transition behavior for elementary particle systems, and a "Mendeleev's table" may be constructed based on the d and n parameters. In such a table, an electron

system would be mapped by the principal quantum number (d) and the orbital angular momentum quantum number (n). Such tables have already been constructed for lattice systems (Fisher, 1974).

iii. Application

The above topological analysis may be extended to random functions in general of the anharmonic oscillator, indicating the relation of fluctuation phenomena to wave events in general.

In the sections above, f corresponds with the momentum, p , and thus for the harmonic oscillator, f corresponds to coordinate x^2 , because $E = hf$ for quantal signals, and $E = 1/2kx^2$ in the case of the harmonic oscillator.

Commencing with the observation that when a particle of mass m and coordinate x acts under the influence of force $F(x) = -x^3 - ax - b$, the equation of motion for such an object is:

$$m\ddot{x} - \eta\dot{x} = -x^3 - ax - b, \quad (101)$$

where η is a damping constant, and a and b are proportionality constants. For convenience, we define a unit mass, i.e., $m = 1$, and denote a/m and b/m by a_0 and b_0 , respectively.

The potential energy of the particle is given by:

$$V(x) = 1/4x^4 + 1/2a_0x^2 + b_0x, \quad (102)$$

as $F(x) = -\partial V/\partial x$. Considering now the case of local stability, we set $x = x = 0$, or

$$x^3 + a_0x + b_0 = 0. \quad (103)$$

The positions of stability, which are determined by the parameters a_0 and b_0 , are thus obtained from Equ. (103).

If $b = 0$, and $a < 0$, the particle has distinct stable positions at either $x_1 = +\sqrt{-a_0}$, or $x_2 = -\sqrt{-a_0}$, as shown in Fig. 30. If a_0 is changed from $a_0 < 0$ to $a_0 = 0$, the two stable positions merge into one at $x_3 = 0$.

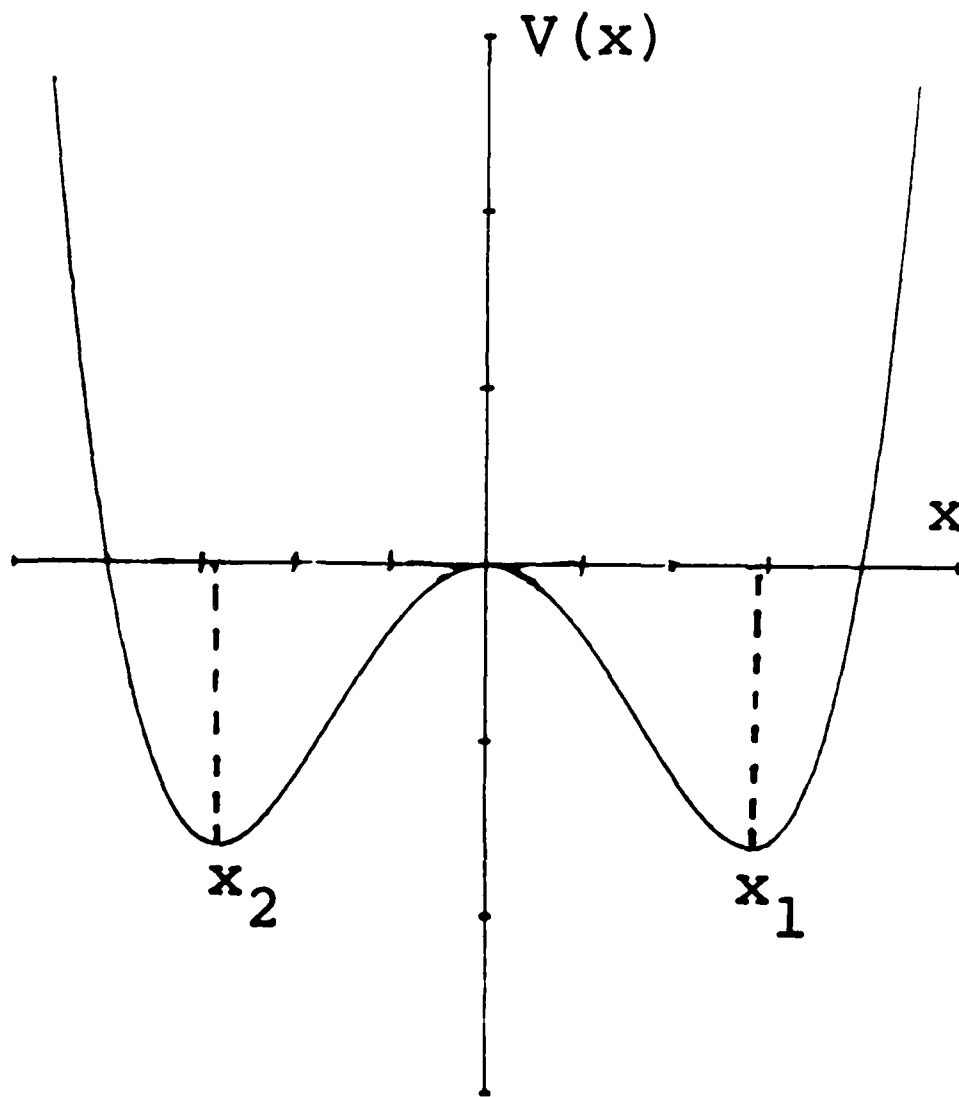


Fig. 30 Potential $V(x) = 1/4x^4 + 1/2ax^2 + bx$ for $b = 0$ and $a < 0$.

Mathematically, a stable position satisfies the condition of minimum potential energy. For the stable positions x_1 and x_2 and $b = 0$, that minimum would be $V(x_{1,2}) = 1/4 a_0^2$, and in the case of a particle confined to the area of instability, $\partial V^2 / \partial x^2 > 0$, and the particle's position would be defined by $x > \pm \sqrt{-a_0/3}$.

We assume now that the particle is located near the origin and its fluctuations into either position, x_1 and x_2 , describable by a random impulse train:

$$\xi(t) = \sum_{i=1}^{\infty} (-1)^J \varepsilon_i \delta(t - t'), \quad (104)$$

where ε_i are the magnitudes, J is either zero or one, and $\delta(t - t')$ is the Dirac delta function. The correlation function of the impulse is then:

$$\langle \xi(t) \xi(t') \rangle = c_0 \delta(t - t'), \quad (105)$$

where c_0 is the magnitude of the impulse at $(t - t')$, the mean time between impulses. It follows that the probability of finding the particle between coordinate x and $x + dx$ at time t is described by the stochastic equation (Sveshnikov, 1968):

$$\dot{f}(x) = \sum_{j=1}^{\infty} \frac{1}{j!} \frac{\partial}{\partial x}^j [k_j(x) f(x)]. \quad (106)$$

Since we are interested here in the simple case of continuous Markov processes, we set $k_3 = k_4 = \dots = 0$, and obtain from Equ. (106) the Fokker-Planck equation:

$$\dot{f}(x) = -\frac{\partial}{\partial x} [k_1(x) f(x)] + 1/2 \frac{\partial^2}{\partial x^2} [k_2(x) f(x)], \quad (107)$$

where $k_1(x)$, $k_2(x)$ are the drift coefficient and the diffusion coefficient respectively. In the present case, $k_1(x)$ is the force defined:

$$k_1(x) = -x^3 - a_0 x - b_0 = -\frac{\partial V}{\partial x}, \quad (108)$$

and the magnitude of the impulse, $k_2(x)$, is:

$$k_2(x) = c_0. \quad (109)$$

We note in passing that this Fokker-Planck equation has been related to birth-and-death descriptions of fluctuations (Nicolis and Prigogine, 1977: Nitzan, Ortoleva, Deutch and Ross, 1973).

We now impose the assumption that the distribution function is normalizable and vanishes at infinity. With the particle in the stationary state, $\dot{f}(x) = 0$, and substituting Eqs. (108) and (109) into (107), we may solve for f with respect to this stationary state and obtain:

$$f(x) = N \exp \left\{ -\frac{2}{c_0} (1/4 x^4 + 1/2 a_0 x^2 + b_0 x) \right\}, \quad (110)$$

where N is a normalization constant.

In the case of $b_0 = 0$, the distribution function, f , can be expressed by a Gaussian wave form:

$$f(x) = N_0 \exp \left\{ -\frac{x^2 - a_0}{2c_0} \right\}, \quad (111)$$

where $n_0 = N \exp \left(\frac{a_0^2}{2c} \right)$ and a_0 and c_0 are mean and variance, respectively.

Equ. (111) may now be compared with the previous result (Eqs. (69)) if the following replacements are made:

$$x^2 \rightarrow f, \quad a_0 \rightarrow \sqrt{a} = f_0 \quad \text{and} \quad 1/2c_0 \rightarrow c(\pi)^2.$$

Transferring the distribution function, $f(x)$, into the frequency domain gives:

$$S(f) = n_0 \exp \{ -c(\pi)^2 (f - f_0)^2 \}, \quad (112)$$

previously obtained (Equ. (71)).

Considering now a particle fluctuating from stable coordinates x_s to a new coordinate $x_s + \delta x$, then if the higher orders of δx are discarded, a new distribution function at $x_s + \delta x$ may be calculated from Equ. (110):

$$f(x_s + \delta x) = N_0 \exp \left[-\left\{ \frac{2}{c_0} \left(\frac{1}{4} x_s^4 + \frac{1}{2} a_0 x_s^2 + b_0 x_s \right) + \frac{1}{c_0} (3x^2 + a_0) \partial c \right\} \right] \quad (113)$$

The particle is then confined to a new position of instability described by the second term of the exponent in Equ. (13): $-(3x_s^2 + a_0)/c_0$. On the other hand, from the $V(x)$, x relation, we know that $\frac{\partial^2 V}{\partial x^2} = 3x_s^2 + a_0$. By imposing the condition of instability, $\frac{\partial^2 V}{\partial x^2} = 0$ at $x = x_s$, $b_0 = 0$, we arrive at the equation for the cusp in the a_0, b_0 plane: $4a_0^3 + 27b_0^2 = 0$, as shown in Fig. 31. The particle may fluctuate on either the positive or negative side of the x axis and along the a_0 axis to $a_0 = 0$. If the restriction $b_0 = 0$ is lifted, the particle may fluctuate on either side of the b_0 axis and along the a_0 axis to $a_0 = 0$.

The circumstance of isomerization in transpolyacetylene (or isomerization in general) is thus related to symmetry breaking in critical phenomena. This is a necessary, but insufficient, condition for dynamic propagation to occur. A further condition is that an energy gap be created between the isomerized states. The creation of this gap was addressed by Hubbard (1963, 1964a,b).

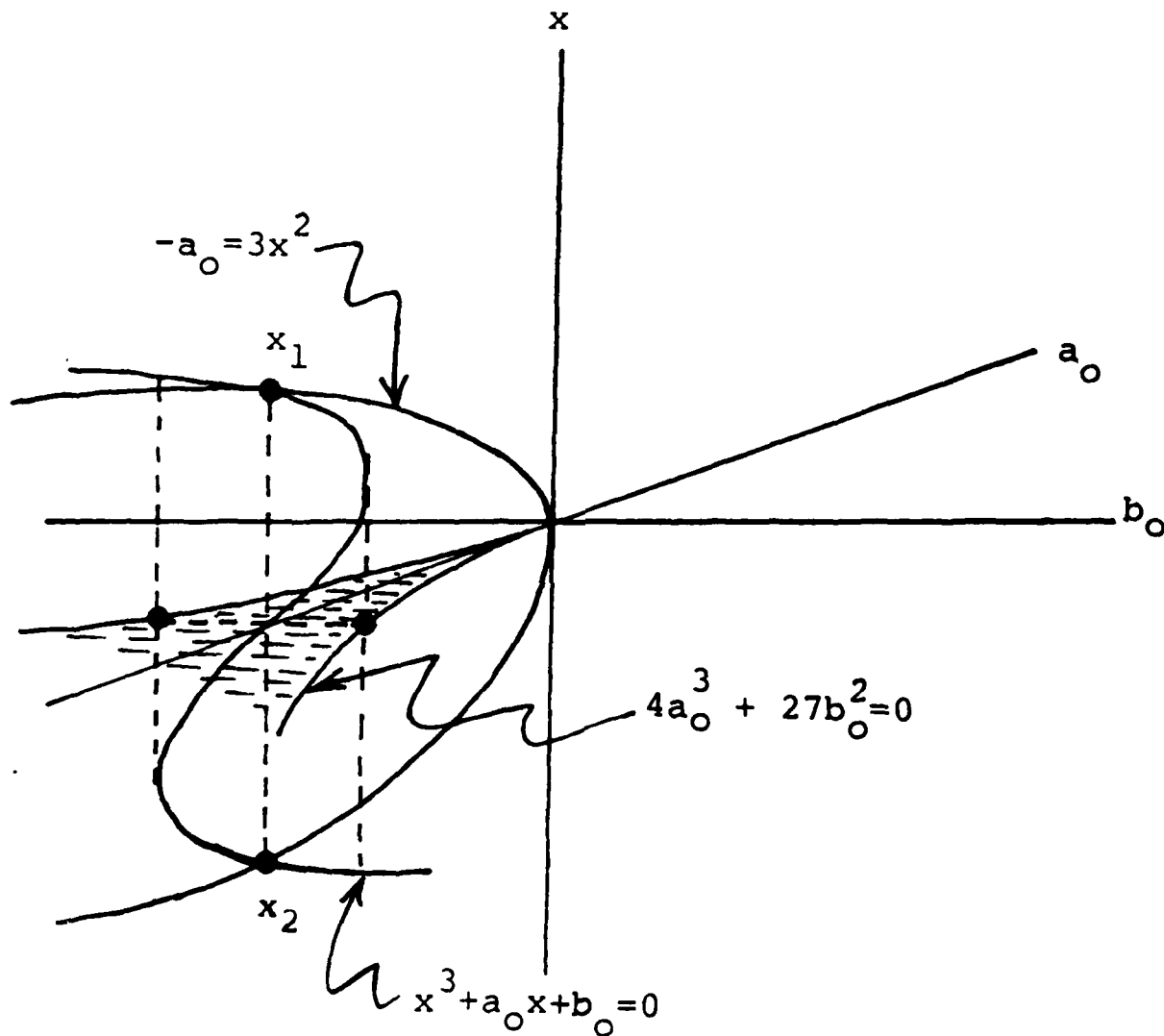


Fig. 31 Fluctuation limits of particle: in the x, b_0 plane ($x^3 + a_0 x + b_0 = 0$; $a_0 < 0$; $b_0 < \pm 1.31$); in the x, a_0 plane ($-a_0 = 3x^2$); and in the a, b_0 plane ($4a_0^3 + 27b_0^2 = 0$).

XI THE HUBBARD MODEL

In sections I - IX soliton propagation was related to exciton-phonon coupling in a one-dimensional system with incommensuration. The

incommensuration permitted an energy gap to develop which established the conditions for parametric excitation diffusion. The soliton propagation was treated microscopically, i.e., each link in the one-dimensional chain was allocated a pump, signal and idler.

Although this approach is necessary and provides physical insight, a macroscopic picture provides empirically a simpler treatment. In essence, this means the replacement of a many-body system by a system of independent quasiparticles moving in a properly determined field which may be random (Economou, White and DeMarco, 1978). Just as Hubbard proposed substituting for a partly filled d-band of noninteracting electrons the total spin of the atom based on correlated electron motions, so one may substitute for the individual monomer units of a one-dimensional conductor, a macroscopic picture of the whole chain, or at least chain parts - if correlations of exciton-phonon coupling are strong enough. Although one may still suppose the microscopic soliton to move from monomer to monomer as described in section I - IX, its motion may be correlated in such a manner as to give properties of a macroscopic theory. Such correlations are describable in terms of Zubarev's (1960) Green's function technique.

Hubbard's model may be viewed quite generally. Just as Hubbard had in mind the case of d-electrons, yet addressed the case of an s-band having two states per atom, so we shall keep in mind the two isomerized states of transpolyacetylene, while yet addressing the general case described by Equ. (62b) which is Equ. (20).

The system addressed by Hubbard behaves as though it has two energy levels T_0 and $T_0 + I$ containing $1 - 1/2n$ and $1/2n$ states per atom, respectively, where I is the interaction energy. Here, on the other hand, a

system of two states are addressed, both of energy T_0 , but for which energy I is needed, if it is to pass from one state to the other. This I , then, is the applied current, I , of Table I of section II or the pumping energy. Given these identifications, there is a direct analogy with the s-band problem and the results of the previous analysis by Hubbard may be adopted.

Proceeding directly, then, to certain conclusions drawn from the Hubbard formulation: if P is the density of states of the band structure (e.g., of the atom or of the whole $(CH)_x$ chain), and p is the density of states of the microsystems (e.g., the electrons or the $(CH)_x$ monomers), then the function $g(E)$ which transforms the microdensity into the macrodensity, $\rho(E) = P(g(E))$, is (Hubbard, 1963, p. 252):

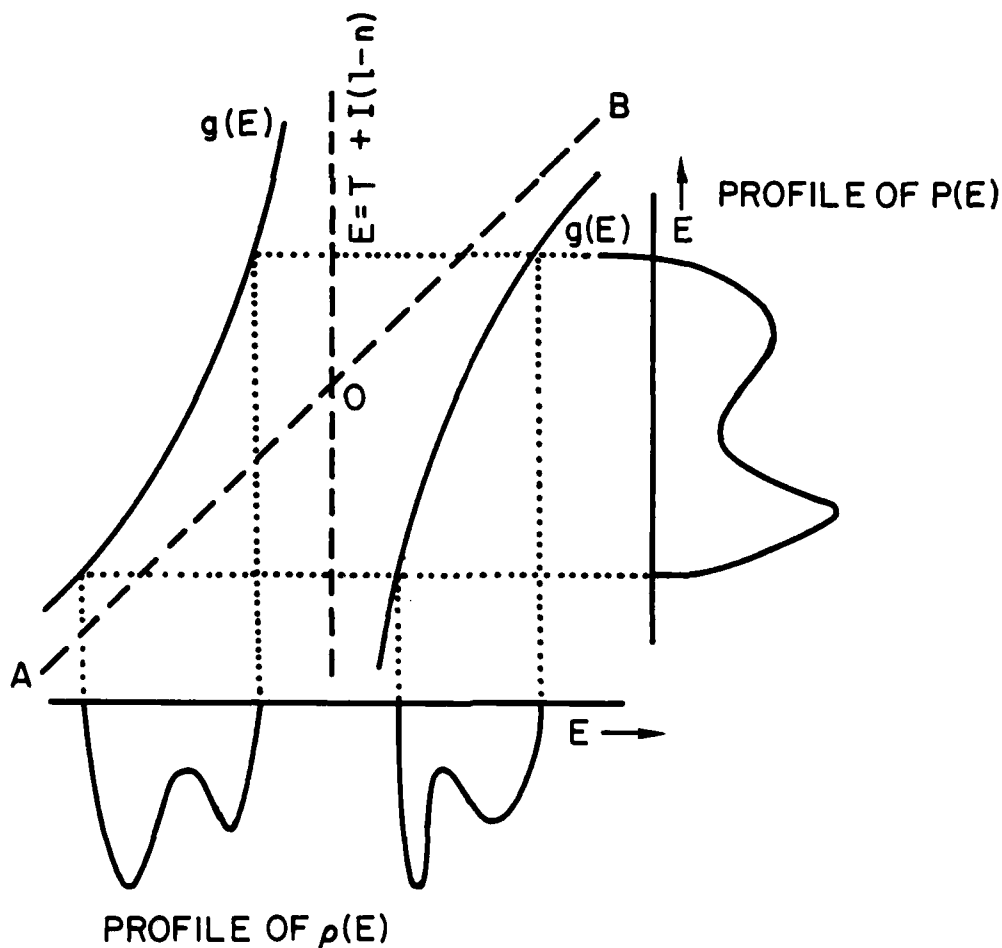


Figure 32: Typical $g(E)$ curve. From Hubbard, 1964, p. 253.

By this relation we see that the band is split into two parts by the infinity of $g(E)$ at $E = T_0 + I(1 - n_{-\sigma})$, where $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ and $c_{i\sigma}^+$ and $c_{i\sigma}$ are creation and destruction operators for electrons - or conformational states in the case of $(CH)_x$ - in the state (i, σ) $\sigma = +1$.

As in the limit, $I \rightarrow 0$, $g(E)$ is the straight line AOB, the splitting of the microdensity of states is due to the perturbation I . This perturbation thus performs the same function as the Peierls distortion in the $(CH)_x$ system or the torsion-bar spring constant, K , of Table I in section II.

Some correspondences with the Hubbard formulation may now be indicated. If $\phi_\mu(x)$ are the degenerate wave functions of $(CH)_x$, μ is a label distinguishing various degenerate wave functions, $c_{i\mu}$ is the destructive operator for a soliton in the state μ on the monomer labeled i , i.e., for a soliton in the state $\phi_\mu(x/R_i)$ where R_i is the position vector of monomer i and $c_{i\mu}^+$ is the corresponding creation operator, then for narrow energy bands the Hamiltonian is (Hubbard, 1964, p. 240):

$$H = \sum_{ij} \sum_{\mu\nu} T_{ij}^{\mu\nu} c_{i\mu}^+ c_{j\nu} + 1/2 \sum_{i,j,k,\ell} \sum_{\mu,\nu,\sigma,\tau} (i,\mu,j | 1/r | k\sigma,\ell\tau) c_{i\mu}^+ c_{j\nu}^+ c_{\ell\tau} c_{k\sigma}, \quad (114)$$

where

$$T_{ij}^{\mu\nu} = \int \phi_\mu^*(x - R_i) \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \phi_\nu(x - R_j) dx, \quad (115)$$

and

$$(i\mu, j\nu | 1/r | k\sigma, \ell\tau) = \frac{e^2 \int \phi_\mu^*(x - R_i) \phi_\sigma(x - R_k) \phi_\nu^*(x - R_j) \phi_\tau(x - R_\ell) dx dx^1}{|x - x^1|} \quad (116)$$

Recalling Equ. (113) above, noting the formal similarity of T_{ij}^μ (Equ.

(115)) and $N_0 \exp[-\{\frac{2}{c_0} (1/4x_s^4 + 1/2a_0 x_s^2 + b_0 x_s)\}]$, the second term in Equ. (114) is equated to $\frac{1}{c_0} (3x_s^2 + a_0) (\partial x)^2$. The general result of section X (iii) above is then applicable to the Hubbard model.

It is instructive to dissect the dynamics of the Hubbard model further. For example, if we equate ϵ_k which are the band energies of the Hubbard electron model with the conformational energies of the $(CH)_x$ chain, E_{ki} with the conformational energies of the separate $(CH)_x$ monomers and equate:

$$D_{\mu\tau}(E) = \sum_{p,q} \frac{(p|c_{\mu}|q)}{E+E_p-E_q} \langle [X_{pq}, C_{\tau}^+]_+ \rangle, \quad (117)$$

where $X_{pq} = |1p\rangle\langle q|$, with the transition probabilities from one to the other of the isomerized states of $(CH)_x$, p and q , then the function $F(E) = \epsilon_k^a - T_0 \equiv \frac{1}{D(E)}$ provides a relation of the microsystems (monomers) to the macrosystem (the chain). This relation exists between the density of states $P(E)$ of the macrosystem and the density of states $\rho(E)$ of the microsystems (Hubbard, 1964a, p. 250):

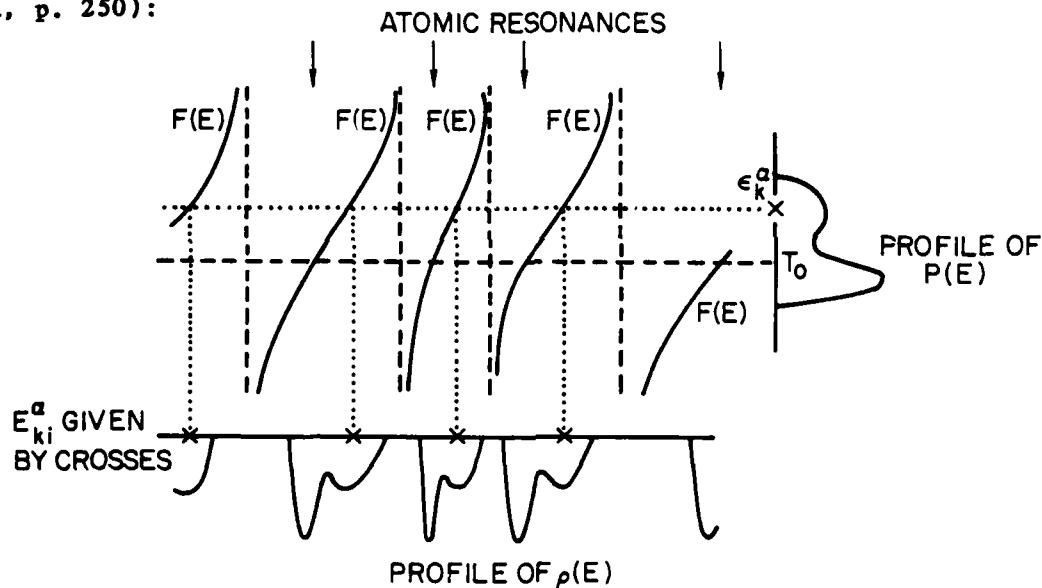


Figure 33: The function $F(E)$ with relation of the density of states $\rho(E)$ and $P(E)$. (Hubbard, 1964a, p. 250).

Clearly, then $F(E)$ is the x of Figures 17 and 22A of section IX and the x of Figure 31 above. As stated in section X (iii) above, this x is a substitution for f_0 of Equ. (62) and the analysis comes full circle.

Equation (62) is also formally similar to the nonlinear Schrödinger equation upon which the Davydov picture of vibrational soliton propagation is built (cf. Davydov and Kislukha (1956) Equ. (16): Davydov (1980a) Equ. (4.4): Davydov (1980b) Equ. (2.22): Davydov and Enol'skii (1980) Equ. (3.2)). Davydov subscribes to the notion, attributed to Fröhlich, that in a one-dimensional system the coupling of electrons with deformation may lead to a superconductive effect without electron coupling. The possibility of such coupling presupposes the creation of an energy gap and Figure 32, above, illustrates the dynamics of the gap's formation.

In this section missing pieces of the puzzle were provided concerning the creation of that necessary gap. Whereas soliton propagation in proteins may require two (vibrational) states separated by an energy gap, I , in the trans $(CH)_x$ system, on the other hand, the two (conformational) states are both of the same energy, but separated by an energy barrier which requires energy, I , to surmount (tunnel through). Given this difference, the soliton propagation picture in its dynamics remains the same.

XII. CONCLUSION

In section X (i) the necessary and sufficient conditions for the obtainment of isomerization in a one-dimensional system were described. In section X (iii) the random functions of an anharmonic oscillator were described, both for the many-body and one-body system. In section XI the one-body (Hubbard) system was described and the obtainment of an energy gap was demonstrated to be formally similar to its obtainment in terms of the anharmonic oscillator picture of section X (iii).

In order to understand the dynamics of the conducting one-dimensional system, a parametric excitation picture was presented in sections I - IX. The advantage of this approach is a physical insight into the dynamics of conduction in $(CH)_x$ type polymers. The disadvantage is that a description of the whole chain in such terms is intractable. On the other hand, in sections X - XI the previous many-body picture was related to the one-body (Hubbard) picture. The advantage of this is that the whole chain becomes quite manageable. The disadvantage is that the dynamics of the problem is only introduced in a quite artificial way (if at all). Clearly, therefore, both pictures are necessary for full understanding.

There is a generalization of this application of the double potential well model to conduction in general in organic polymers. The relationship between one-dimensional theories in field theory and statistical mechanics is of importance in the study of quasi one-dimensional systems due to the relation of the Bethe Ansatz (Bethe, 1931), on the one hand, and the transfer matrix methods of Onsager (1944) and Baxter (1972) on the other (cf. Fowler, 1981; Berkan and Cooper, 1981). In particular, the diagonalization of the Hamiltonian or the transfer matrix has been achieved in all these models by one form or another of the Bethe Ansatz. Also, this

method was used to diagonalize the massive Thirring model (Bergnoff and Thacker, 1979), the Gross-Neveu model (Andrei and Lowenstein, 1979) and the Kondo problem (Andrei, 1980).

Furthermore, recently Campbell and Bishop (1981, 1982a,b; Bishop, 1980) demonstrated the relation of solitons in polyacetylene to relativistic-field-theory models and established the existence within a continuum electron-phonon model, of a polaron-like excitation additional to and different from the amplitude "kink".

The relativistic-field-theory aforementioned is the Gross-Neveu model (Gross and Neveu, 1974) described by a Lagrangian density of anharmonic oscillator type. Polyacetylene exemplifies the situation of a single electron spectrum with two states symmetrically placed in the gap at $\epsilon^{\pm} = \pm w_0$, which exists only when there is a single unpaired electron occupying the ϵ^{-} state, or, when the ϵ^{-} state is only singly occupied by a localized hole state. Since the electron or hole is trapped in a structure due to phonon coupling, the excitation is polaron-like. Similar results have been obtained by Brazovskii (1978, 1980) and Takayama, Lin-Liu and Maki (1980). This continuum model has also been addressed by Horovitz (1980, 1981) and Krumhansl, Horovitz and Heeger (1980).

These developments differ from the Su, Schrieffer and Heeger (1979, 1980) treatment of electrical conduction in polyacetylene in that the soliton-like polarons are obtained from continuum models, whereas Su et al., imposed a hyperbolic tangent (\tanh) kink form on the Pierls amplitude order parameter to obtain kink solutions. Both Brazovskii and Takayama et al., on the other hand, demonstrate that the order parameter profile is an exact solution in the continuum limit of the self-consistent equations of motion for phonon and electron operators determined in a variational scheme. Thus,

this development is fully compatible with the physical scheme represented here.

Campbell and Bishop also point out an exact formal equivalence between the Brazovskii-Takayama et al., continuum equations and the static classical equations of the $N=2$ Gross-Neveu model (Gross and Neveu, 1974; Dashen, Hasslacher and Neveu, 1974c; 1975a,b). By means of the mean field approximation, the Bogliubov-de Gennes equations relating electron and phonon fields were obtained. Dashen et al., demonstrated that there are three classes of solutions to the Gross-Neveu Lagrangian: (1) The ground-state solution; (2) The kink solution; and (3) The "bag" solution involving the presence of fermions in occupied positive energy bound states and the absence of fermions from negative energy bound states in the case of antiparticle or hole excitation. The field trapping the fermion is driven by phonon coupling to the fermion, i.e., the fermion is a polaron.

Also, Zamolodchikov and Zamolodchikov (1978, 1979) demonstrated how to determine the exact S matrices of two-dimensional models including the sine-Gordon equations and the $(\bar{\Psi}\Psi)^2$ model. Witten (1978) determined that the Lagrangian model used may be considered an N -component Majorana Fermi field. For $N=2$ the theory is of a single interacting Dirac field and is, in fact, the massive Thirring model related to soliton theory by Coleman (1975). For $N=3$ the field is equivalent to a supersymmetric sine-Gordon equation and for $N=4$, to two decoupled sine-Gordon systems.

The general anharmonic oscillator model forming the basis of these developments has been most extensively studied by Dashen, et al. Their methods, in turn, are based on those of Gurzwiller (1967, 1970, 1971) and Maslov (1970). The meaning of the WKB approximation was examined from a functional-integral approach and the conclusion was made that certain kinds

of nonlinear field theories have extended particle solutions which survive quantization. Theories with spontaneous symmetry breaking were shown to produce hadron-like objects. In these instances, the field theory becomes a model for a superconductor. Models in four space-time dimensions can be constructed of $SU(2)$ Yang-Mills fields coupled to fermions and a spontaneous-asymmetry-breaking scalar isospinors.

Dashen et al. (1975a) also used the WKB method to compute the particle spectrum of the Gross-Neveu model and found a spectrum of particles of fermion-antifermion bound states and multifermion bound states. The close similarity between the sine-Gordon equation and the Gross-Neveu model was noted, but the reason for the correspondence not discerned. It is, however, probably not unimportant that the Lagrangian for both theories are examples of Riemann-Hugoniot singularities. Dashen et al (1975b) pointed out the correspondence of the sine-Gordon coupling parameter and the four fermion coupling of the Thirring model. The fermions are thus solitons.

In conclusion, therefore, the anharmonic oscillator model, whether in the form of linked pendula model, or conducting polymer form, offers a rich spectrum of particles. Due to the so-called "democracy" of the sine-Gordon equation (Dashen et al 1975b), there is no fundamental distinction between the particle of the $n = 1$ quantum state and the higher mass $n > 1$ particles. As the anharmonic oscillator model indicates electron-phonon coupling involvement in electrical conduction, and the electron can occupy any of those states, one may expect a rich variety of polymers able to conduct either—electrically or vibrationally—besides the one-dimensional. This is because application of the anharmonic oscillator model is appropriate under any condition in which the double potential well model applies.

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